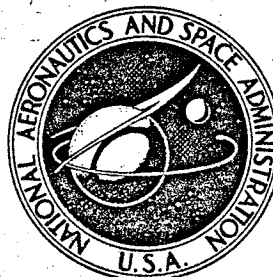


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GENERAL CHEMICAL KINETICS COMPUTER
PROGRAM FOR STATIC AND FLOW REACTIONS,
WITH APPLICATION TO COMBUSTION
AND SHOCK-TUBE KINETICS

by David A. Bittker and Vincent J. Scullin

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16. Abstract <p>A general chemical kinetics program is described for complex, homogeneous ideal-gas reactions in any chemical system. Its main features are flexibility and convenience in treating many different reaction conditions. The program solves numerically the differential equations describing complex reaction in either a static system or one-dimensional inviscid flow. Applications include ignition and combustion, shock wave reactions and general reactions in a flowing or static system. An implicit numerical solution method is used which works efficiently for the extreme conditions of a very slow or a very fast reaction. The report includes a description of the theory and the computer program, including a complete users manual. Information on obtaining the program may be obtained from the authors.</p>		
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GENERAL CHEMICAL KINETICS COMPUTER PROGRAM FOR STATIC AND FLOW REACTIONS, WITH APPLICATION TO COMBUSTION AND SHOCK-TUBE KINETICS

by David A. Bittker and Vincent J. Scullin

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SUMMARY

A general chemical kinetics computer program for complex, homogeneous ideal-gas reactions is described. It is designed for flexibility and convenience in treating reactions under many different conditions. Some of these conditions are (1) reaction behind a shock wave, (2) ignition and combustion reactions in a static or flowing system, (3) combustion and nozzle expansion, and (4) general reaction in a static system or one-dimensional frictionless flow. In any system the temperature or volume or both may be held constant.

An implicit numerical integration method is used for the solution of the differential equations that describe a complex reaction. A new step size optimization procedure has been developed to make this technique work efficiently for a wide range of conditions. This includes the extremes of very slow and very fast reaction.

This report describes the theoretical equations involved, as well as the numerical method of solution. A detailed description of the program is given including preparation of input data, control of accuracy, sample input data, and several examples of test case results.

INTRODUCTION

Chemical kinetics calculations in reacting gases are of interest today for many different applications. Some examples are (1) ignition and combustion of fuel-oxidant mixtures, (2) expansion of combustion products, and (3) chemical reaction behind a shock wave. Very involved numerical methods are needed for detailed computations in a gas where many reactions are occurring at the same time. Simplifying assumptions can

sometimes be made while still obtaining useful results. Some of these for exhaust nozzle flow are discussed in references 1 and 2. Two of the most used ideas are (1) the assumption of equilibrium flow (infinite reaction rates) and (2) the assumption of sudden freezing or rapid transition from infinite reaction rates to zero reaction rates. The assumption (2) often gives useful information with the use of only a small amount of chemical kinetic information. For better insight into the reaction details, however, exact theoretical calculations are needed. The term exact is used here to mean that all important chemical reactions and their rate constants are included in the analysis. The actual solution of the nonlinear set of fluid-dynamic and kinetics equations involves some mathematical simplifications. Treanor (ref. 3) transformed these differential equations into difference equations. Other investigators locally linearized the differential equations by removing second-order terms. They then used either an exact (ref. 4) or an approximate (refs. 5 and 6) analytic solution or finite difference solutions (refs. 7 and 8).

Several computer programs have been written which use a finite difference method to integrate the differential equations of chemical kinetics. The main effort in developing these programs was to make the integration scheme overcome a mathematical instability problem that arises in these calculations. This problem is discussed in detail in a later section of this report. Briefly stated, it is the fact that some integration methods require a very small step size to maintain accuracy and stability when the chemical reaction is either very fast or very slow. This leads to excessively long computation times. The program described in reference 34 uses the technique of reference 3 to avoid these problems. Reference 9 describes rocket performance programs that use the inherently stable implicit integration technique of reference 8. Reference 35 describes another more general kinetics program based on this technique. These and other programs have the ability to handle many types of kinetics problems for many chemical systems. However, no single program has been found that could conveniently be used in a wide variety of flow and static reaction problems for an arbitrary chemical system.

For this reason, a general chemical kinetics computer program for complex gas mixtures has been developed at Lewis. It is written completely in FORTRAN IV, version 13, and was developed on an IBM 7044-7094/direct-couple system. This program can be used for any homogeneous reaction in either a flowing or a static system. It has the advantages of flexibility, accuracy and ease of use. Moreover, any chemical system may be used for which species thermodynamic data and reaction rate constants are known. The program handles several types of reaction. These include bimolecular exchange reactions, unimolecular decompositions, bimolecular decompositions, and the reverse recombination processes. The solution method is a rapid one based on the implicit finite-difference technique of Kliegel and Tyson (refs. 8 and 9). A unique step-size control system is used to estimate the optimum step size for each step. Moreover, the user can easily change the preset program controls to give his own balance between

acceptable accuracy and computing time. For flow reactions this program assumes one-dimensional flow. This is usually a good approximation for systems of practical interest, and the additional complications of three-dimensional kinetics computations (surveyed in ref. 10) are not required.

The purpose of this report is to present a complete description of the chemical kinetics computer program and the implicit numerical integration method it uses. The theoretical kinetics differential equations solved by the program are also given in detail. The program may be used (with either assigned pressure or area in flow reactions) for the following problems:

- (1) Chemical reaction behind a shock wave
- (2) Ignition and combustion in a flowing or static system
- (3) Ignition, combustion, and nozzle expansion in supersonic flow
- (4) Chemical reaction in any flowing gas mixture whose velocity does not reach the velocity of sound
- (5) Chemical reaction in any static system
- (6) Constant temperature and/or constant volume reactions

Readers interested primarily in using the program should read the section GENERAL DESCRIPTION OF PROGRAM USE for a description of program options, species information, and accuracy control. A detailed program users manual and computed test case results are given in appendixes. Further information on availability of the program may be obtained from the authors.

SYMBOL LIST

General:

A	area
A_1, A_2, \dots, A_7	thermodynamic coefficients in eqs. (81) to (84)
\mathcal{A}	species production function defined by eq. (12), sec^{-1}
\mathcal{A}^*	\mathcal{A}/V
\mathcal{B}	enthalpy production function defined by eq. (13), sec^{-1}
\mathcal{B}^*	\mathcal{B}/V
C_p	heat capacity of gas per unit mass assuming constant composition (defined by eq. (16))
D	shock tube hydraulic diameter used to calculate L_m (eq. (80)), cm
$F(\mathcal{F}, P)$	shock pressure function defined by eq. (A13)

$G(\mathcal{T}, P)$	shock enthalpy function defined by eq. (A14)
G	Gibbs free energy
H_c	total mixture energy per unit mass
h	total mixture static enthalpy per unit mass
h_1	mixture static enthalpy per unit mass before passage of shock wave
h^*	enthalpy function defined by eq. (A12)
l	number of chemical reactions
L_m	characteristic shock tube reaction length in eq. (80), cm
M	mixture Mach number defined by eq. (14)
M_w	mixture molecular weight
\dot{m}	mass flow rate
N	number of species in a gas mixture
P	p/p_1
p	absolute pressure of gas mixture
p_1	pressure before passage of a shock wave
q	independent variable, either t or x
R	universal gas constant
r	density (ρ) if time is the integration variable; or mass flux (ρV) if distance is the integration variable
S	entropy
S_1	species production function defined by eq. (C37)
S_2	enthalpy production function defined by eq. (C38)
T	absolute temperature
T_0	reference temperature for calculating individual species enthalpy
T_1	temperature before passage of a shock wave
\mathcal{T}	T/T_1
t	time
V	velocity
V_S	shock speed
X_H	total energy exchange rate defined by eq. (86)

x	distance coordinate
β	boundary-layer parameter used to calculate L_m in eq. (80)
γ	specific heat ratio defined by eq. (15)
η	exponent in shock boundary-layer equation (eq. (80))
μ	gas viscosity used to calculate L_m (eq. (80))
ρ	density
ρ_1	density before passage of shock wave

Subscripted Thermochemical Symbols:

In general subscript i refers to species i and subscript j to reaction j . In the appendixes other indexes are sometimes used to avoid confusion in the summations, but their meaning should be clear.

A_j	preexponential constant in the rate constant equation (eq. (33))
$(C_p)_i$	molar heat capacity of species i in a mixture
E_j	activation energy in rate constant equation (eq. (33)), cal/mole
h_i	static molar enthalpy of species i
K_j	equilibrium constant defined by eq. (34)
k_j	forward reaction rate constant (see eq. (32)); units are either $\text{cm}^3 \text{ mole}^{-1} \text{ sec}^{-1}$ or $\text{cm}^6 \text{ mole}^{-2} \text{ sec}^{-1}$ depending on the type of reaction
M_j	third-body efficiency factor defined by eq. (38)
m_{ij}	third-body efficiency ratio of species i in reaction j defined by eq. (39)
n_j	temperature exponent in rate constant equation (eq. (33))
S_i	entropy of species i , energy per mole K
S_1, S_2, \dots, S_N	symbols for species names in general reaction, (eq. (32))
W_i	net species production rate, $\text{moles vol}^{-1} \text{ sec}^{-1}$
X_j	net conversion rate $(\text{mole vol}^{-1} \text{ sec}^{-1})/(\text{density})^2$
$X_{H,j}$	net energy exchange rate, defined by eq. (43)
$\nu_{i,j}$	forward stoichiometric coefficient in general reaction (eq. (32))
$\nu'_{i,j}$	reverse stoichiometric coefficient in general reaction (eq. (32))
σ_i	concentration, moles of species i per unit mass of mixture

$\omega_{i,j}$ net rate of formation of i^{th} species in j^{th} reaction, moles $\text{vol}^{-1} \text{sec}^{-1}$

Subscripted Symbols for Numerical Computation:

In these symbols i and j refer to a particular dependent variable, and n refers to a finite difference step. Exceptions are made in the text for some summations, but the interpretation is obvious. The independent variable is shown here as t , but the same notation applies if x is used.

C	step-size ratio defined in eq. (69)
$D_{i,n}$	ratio of increment to step size defined by eq. (70)
$E_{i,n+1}$	relative error in y_i at time $t = t_{n+1}$ defined by eq. (62)
f_i	dy_i/dt
$f_{i,n}$	dy_i/dt at $t = t_n$
h_n	$t_n - t_{n-1}$
h_1	$t_1 - t_0$
h_{max}	maximum step size
h_{min}	minimum step size
$I_1, I_2, \text{ etc}$	intervals of uncertainty in step size search procedure
$k_{i,n}$	$y_i(t_n) - y_i(t_{n-1})$
$k_{i,n}^{(e)}$	exact value of $k_{i,n}$
t_n	time at the n^{th} step
t_0	initial time
y_i or y_j	general dependent variable
$y_{i,n+1}$	$y_i(t)$ at $t = t_{n+1}$
α_i	$\partial f_i / \partial t$
$\alpha_{i,n}$	$\partial f_i / \partial t$ at $t = t_n$
$\beta_{i,j}$	$\partial f_i / \partial y_j$
$\beta_{i,j,n}$	$\partial f_i / \partial y_j$ at $t = t_n$
ϵ_{n+1}	relative error in complete solution at $(n+1)^{\text{st}}$ step, see eq. (72)
ϵ_{max}	maximum relative error per step

FLUID DYNAMIC AND CHEMICAL EQUATIONS

Differential Equations for Assigned Area

The conservation equations for a complex reacting gas are presented in this section. (See, for example, the book by Penner, ref. 11). They are derived first for one-dimensional steady-state flow through an arbitrarily assigned area profile.

Global mass conservation is given by the equation

$$\rho AV = \dot{m} \quad (1)$$

or

$$\frac{d\dot{m}}{dt} = 0 \quad (1a)$$

where \dot{m} is the constant mass flow rate of the gas. Individual species continuity equations for the N species in the mixture are written as

$$\frac{d}{dt} (\sigma_i \dot{m}) = W_i AV \quad i = 1, 2, \dots, N \quad (2)$$

Here σ_i is the number of moles of species i per unit mass of mixture. Expressions for the species production rates, W_i will be given in a following section. By performing the indicated differentiation in equation (2) and using equations (1) and (1a) the following set of equations can be obtained

$$\frac{d\sigma_i}{dt} = \frac{W_i}{\rho} \quad i = 1, 2, \dots, N \quad (3)$$

To completely describe the system we assume adiabatic flow of an ideal gas and neglect viscosity, diffusion and heat conduction. The following additional equations can then be written for momentum and energy conservation

$$\rho \frac{dV}{dt} + \frac{1}{V} \frac{dp}{dt} = 0 \quad (\text{momentum}) \quad (4)$$

$$h + \frac{V^2}{2} = H_c \quad (\text{energy}) \quad (5)$$

where H_c is the total, constant energy of the gas per unit mass and h is the static enthalpy per unit mass of the gas given by

$$h = \sum_{i=1}^N \sigma_i h_i \quad (6)$$

$$h_i = (h_i)_{T_0} + \int_{T_0}^T (C_p)_i dT \quad (6a)$$

Here h_i is the molar enthalpy of species i .

The molecular weight of the gas mixture is

$$M_w = \frac{1}{\sum_{i=1}^N \sigma_i} \quad (7)$$

The equation of state is

$$p = \frac{\rho RT}{M_w} \quad (8)$$

Equations (1), (5), (7), and (8) are differentiated and combined with equation (4) to get the following differential equations:

$$\frac{dV}{dt} = \frac{V}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dt} - \mathcal{A} \right) \quad (9)$$

$$\frac{d\rho}{dt} = -\rho \left[\frac{M^2}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dt} - \mathcal{A} \right) + \mathcal{A} \right] \quad (10)$$

$$\frac{dT}{dt} = -T \left[\frac{(\gamma - 1)M^2}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dt} - \mathcal{A} \right) + \mathcal{B} \right] \quad (11)$$

In these equations the following auxiliary definitions have been made:

$$\mathcal{A} = \frac{RT}{p} \sum_{i=1}^N w_i - \mathcal{B} \quad (12)$$

$$\mathcal{B} = \frac{1}{p} \left(\frac{\gamma - 1}{\gamma} \right) \sum_{i=1}^N h_i w_i \quad (13)$$

$$M^2 = \frac{V^2 M_w}{\gamma RT} \quad (\text{definition of Mach number}) \quad (14)$$

$$\gamma = \frac{C_p}{C_p - \frac{R}{M_w}} \quad (15)$$

$$C_p = \sum_{i=1}^N \sigma_i (C_p)_i \quad (16)$$

where C_p is the heat capacity of the mixture per unit mass assuming fixed composition and $(C_p)_i$ is the molar heat capacity of species i . Equations (3), and (9) to (11) form a system of $N + 3$ equations in $N + 3$ unknowns. Their solution must be obtained by a numerical technique.

The equations for a static reaction can now be obtained by setting the velocity equal to zero in equations (9) to (11) to get the system

$$\frac{d\sigma_i}{dt} = \frac{W_i}{\rho} \quad i = 1, 2, \dots, N \quad (3)$$

$$\frac{d\rho}{dt} = -\rho\mathcal{A} \quad (17)$$

$$\frac{dT}{dt} = -T\mathcal{B} \quad (18)$$

The reacting gas can also be described by equations that use distance, x as the independent variable. The relation $dQ/dx = (1/V)dQ/dt$ is used to rewrite equations (3), (9), (10), and (11). Here Q represents any of the variables V , ρ , T , or σ_i . The new equations are

$$\frac{d\sigma_i}{dx} = \frac{W_i}{\rho V} \quad i = 1, 2, \dots, N \quad (19)$$

$$\frac{dV}{dx} = \frac{V}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dx} - \mathcal{A}^* \right) \quad (20)$$

$$\frac{d\rho}{dx} = -\rho \left[\frac{M^2}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dx} - \mathcal{A}^* \right) + \mathcal{A}^* \right] \quad (21)$$

$$\frac{dT}{dx} = -T \left[\frac{(\gamma - 1)M^2}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dx} - \mathcal{A}^* \right) + \mathcal{B}^* \right] \quad (22)$$

where

$$\mathcal{A}^* = \frac{\mathcal{A}}{V} \quad (23)$$

and

$$\mathcal{B}^* = \frac{\mathcal{B}}{V} \quad (24)$$

The derivations so far have assumed adiabatic reaction. To consider instead a constant temperature reaction it is only necessary to set dT/dt or dT/dx equal to zero. This can be shown to be equivalent to eliminating the adiabatic energy equation (eq. (5)). The same situation holds if volume (or density) is held constant in a static reaction. The density derivative, $d\rho/dt$ or $d\rho/dx$, is set equal to zero to obtain the solution for a static reaction at constant volume. Both temperature and volume can also be held constant simultaneously.

Differential Equations for Assigned Pressure

In the equations just derived the flow area is arbitrarily assigned. The pressure is computed from the equation of state (eq. (8)) after density, temperature, and composition have been computed from the differential equations (9) to (11). For engine combustor modeling it is often useful to reverse this procedure. One assigns a desired pressure profile and computes the area profile which then satisfies all the fundamental kinetics and fluid dynamics laws. For this type of calculation another set of differential equations can be derived to replace equations (9) to (11). The derivatives of the dependent variables are now expressed in terms of p and dp/dt rather than A and dA/dt . The new equations, obtained from equation (4) and by differentiating equations (5), (7), and (8), are as follows:

$$\frac{dV}{dt} = -\frac{1}{\rho V} \frac{dp}{dt} \quad (25)$$

$$\frac{d\rho}{dt} = \rho \left(\frac{1}{\gamma p} \frac{dp}{dt} - \mathcal{A} \right) \quad (26)$$

$$\frac{dT}{dt} = T \left[\left(\frac{\gamma - 1}{\gamma} \right) \frac{1}{p} \frac{dp}{dt} - \mathcal{B} \right] \quad (27)$$

The quantities \mathcal{A} and \mathcal{B} are the same as previously defined in equations (12) and (13). If distance, x is the independent variable, the assigned pressure equations are the same, with dp/dt replaced by dp/dx and \mathcal{A} and \mathcal{B} replaced by \mathcal{A}^* and \mathcal{B}^*

$$\frac{dV}{dx} = -\frac{1}{\rho V} \frac{dp}{dx} \quad (28)$$

$$\frac{d\rho}{dx} = \rho \left(\frac{1}{\gamma p} \frac{dp}{dx} - \mathcal{A}^* \right) \quad (29)$$

$$\frac{dT}{dx} = T \left[\left(\frac{\gamma - 1}{\gamma} \right) \frac{1}{p} \frac{dp}{dx} - \mathcal{B}^* \right] \quad (30)$$

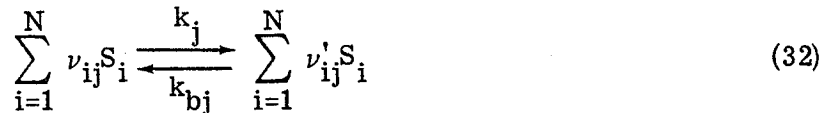
Either of these equation sets is solved (along with the appropriate equations for $d\sigma_i/dt$ or $d\sigma_i/dx$) to give V , T , ρ , and the σ_i 's. Then area is computed from the assigned constant mass flow rate using the mass conservation equation, equation (1).

Chemical Reaction Equations and Species Production Rates

The species formation rate, W_i that appears in equations (3) and (19) is given by

$$W_i = \sum_{j=1}^l \omega_{ij} \quad (31)$$

where l is the number of chemical reactions occurring and ω_{ij} is the net rate of formation of species i by the j^{th} reaction in moles per unit volume per second. Each chemical reaction is written in general form as



where S_i is the i^{th} species. The ν_{ij} and ν'_{ij} are the forward and reverse stoichiometric coefficients for S_i and k_j and k_{bj} are the forward and reverse rate constants for the j^{th} reaction. Each k_j is a function of temperature given by the equation

$$k_j = A_j T^{n_j} e^{-E_j/RT} \quad (33)$$

The value of k_{bj} is calculated from k_j and the equilibrium constant K_j (in concentration units) by the law of microscopic reversibility

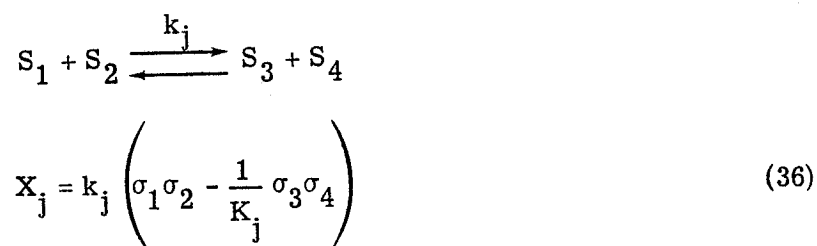
$$k_{bj} = \frac{k_j}{K_j} \quad (34)$$

For convenience we introduce the net reaction conversion rate X_j which is related to ω_{ij} by the equation

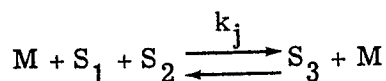
$$\omega_{ij} = \rho^2 (\nu'_{ij} - \nu_{ij}) X_j \quad (35)$$

The units of X_j are (moles/vol sec)/(density)². It is useful as a measure of the amount of change due to each reaction occurring in the gas mixture. We use X_j rather than the net molar reaction rate because the X_j values are more convenient for comparison than the molar rates. The exact form of X_j depends on the type of reaction being considered. In this program three types of reversible chemical reaction are considered. These reactions and the corresponding X_j formulas are given next.

Type 1 - bimolecular shuffle reaction:



Type 2a - three-body recombination:



where M , the catalyst molecule, can be any species present.

$$X_j = k_j M_j \left(\rho \sigma_1 \sigma_2 - \frac{\sigma_3}{K_j} \right) \quad (37)$$

where M_j , the third-body efficiency factor for the j^{th} reaction is

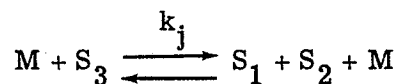
$$M_j = \sum_{i=1}^N m_{ij} \sigma_i \quad (38)$$

In this equation m_{ij} is the third-body efficiency factor for species i in the j^{th} reaction. It is a correction only on the preexponential factor A_j in equation (33) and can be written as

$$m_{ij} = \frac{(A_j)_{\text{species } i}}{(A_j)_0} \quad (39)$$

where $(A_j)_0$ is the A_j value for a reference species as a third body.

Type 2b - two-body dissociation:

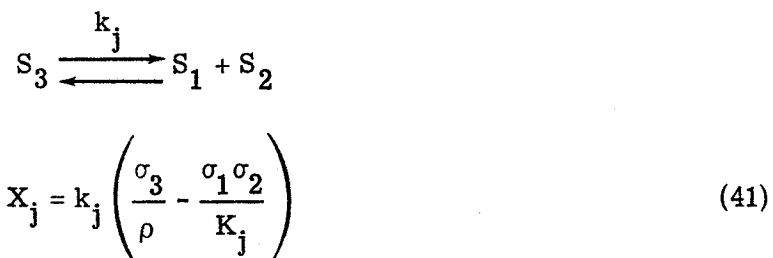


where M is the catalyst molecule

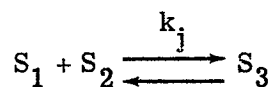
$$X_j = k_j M_j \left(\sigma_3 - \frac{\rho \sigma_1 \sigma_2}{K_j} \right) \quad (40)$$

where M_j is defined by equation (38).

Type 3a - unimolecular decomposition:



Type 3b - two-body recombination:



$$X_j = k_j \left(\sigma_1 \sigma_2 - \frac{\sigma_3}{\rho K_j} \right) \quad (42)$$

The size of X_j tells approximately the importance of any single reaction among all those occurring. The sign of X_j tells how the reaction is actually occurring: X_j is positive if the j^{th} reaction is proceeding from left to right as written, and negative if it is proceeding in the opposite direction.

For some problems the heat release rate is an important consideration. For such situations another useful quantity was defined and used in reference 12 to measure a reaction's importance. This is the net energy conversion rate for the j^{th} reaction defined by

$$X_{H,j} = X_j (\Delta H_{298})_j \quad (43)$$

where $(\Delta H_{298})_j$ is the molar heat of reaction at 298 K for the j^{th} reaction proceeding in the forward direction, from left to right.

Normal Shock Equations

A chemical reaction can be started by the passage of a shock wave through a gas. The assumption is made that the shock wave instantaneously raises the gas to new temperature and pressure conditions without changing its composition. The conservation equations for the change in conditions across the shock are

$$\rho_1^2 V_S^2 = \rho^2 V^2 \quad (44)$$

$$p_1 + \rho_1 V_S^2 = p + \rho V^2 \quad (45)$$

$$h_1 + \frac{V_S^2}{2} = h + \frac{V^2}{2} \quad (46)$$

In these equations the coordinate system is attached to the shock, which is considered stationary. The unshocked gas at conditions p_1 , ρ_1 , and T_1 flows past the shock with speed V_S , the experimental shock velocity. Gas properties immediately after the shock passes are p , ρ , and T . The enthalpy per gram of gas mixture is changed from h_1

to h by the shock. Since gas composition is unchanged, h is calculated for the initial composition at the new temperature T . The actual equations solved are given in appendix A. These conditions are called the no-reaction or frozen shock conditions.

The increased temperature and pressure behind the shock start the chemical reaction. It is also possible to solve equations (44) to (46) for the equilibrium postshock conditions. These are the final velocity, temperature, pressure, and new composition that would exist after all chemical reaction is complete. The solution method for this situation is also described in appendix A. The complete shock-equation solution uses the method described by Gordon and McBride (ref. 13).

NUMERICAL ANALYSIS

Summary of Technique

The nonlinear, coupled differential equations derived in the previous section (e.g., eqs. (19) to (22)) describe the relaxation of a reacting gas toward equilibrium. The relaxation rates of the fluid mechanical variables are often quite different from the relaxation rates of the component gases, particularly in near-equilibrium flow regimes. In addition, there can be large differences in the relaxation rates of the individual gases. Systems of differential equations which represent relaxation processes with widely different relaxation rates are called stiff systems.

The numerical integration of a system of stiff differential equations poses a serious stability problem. The problem arises in trying to resolve rapid variations over the small regions in which they contribute significantly to the solution while at the same time advancing the integration at a rate which is consistent with the slower, more dominant solutions. Most conventional numerical integration techniques force the step size to be impractically small in order to maintain stability.

Many integration techniques have been derived which are both more stable and more efficient than conventional methods for integrating stiff systems. Among these are Treanor's modified Runge-Kutta method (ref. 3) and Moretti's method (ref. 4) involving the exact solution of locally linearized equations. A method which falls logically between those two is the implicit integration method of Tyson (refs. 8 and 14). This method has the advantages of being inherently stable and computationally efficient. The inherent stability of Tyson's method makes it preferable for general applications where nothing is known ahead of time about the disparity in relaxation rates (see ref. 15). The general chemical kinetics program uses the implicit integration method of Tyson with modifications to the initial step and error formulas. Other inherently stable implicit integration methods have been proposed by Lomax and Bailey (ref. 7) and Liniger and Willoughby (ref. 16).

Since Tyson's method is stable for all step sizes, the stability problem is solved. However, the gain in stability obtained by using an implicit rather than an explicit integration method is accomplished at the expense of increasing the number of calculations that must be performed at each step. In particular, all the implicit schemes mentioned require the calculation of all the partial derivatives of the differential equations (see appendixes B and C). The application of an effective strategy for step-size control can significantly increase the rate at which the numerical integration advances. The general chemical kinetics program uses a step-size optimization procedure that is superior to the standard doubling and halving method of step-size control. After each step of the numerical integration, an error predictor is used to search within limits for the largest step size that can be used for the next step without violating the user's accuracy requirements. Experience has shown that this optimization technique permits the step size to react quickly to regions of very slow or very fast reaction.

Derivation of Numerical Integration Equations

This section presents a complete derivation of Tyson's general step formula (ref. 14) and our initial step and error formulas. A derivation of Tyson's formula for a fixed step size is contained in reference 9.

General step formula. - Let the following set of coupled first-order simultaneous differential equations be given:

$$\frac{dy_i}{dt} = f_i(t, y_1, y_2, \dots, y_N) \quad i = 1, 2, \dots, N \quad (47)$$

It will be assumed that these equations are nonsingular and that a solution exists which can be developed as a Taylor series. In other words, for $|t_{n+1} - t_n|$ sufficiently small,

$$k_{i,n+1} = \left. \frac{dy_i}{dt} \right|_{t_{n+1}} h_{n+1} - \left. \frac{d^2 y_i}{dt^2} \right|_{t_{n+1}} \frac{h_{n+1}^2}{2!} + \left. \frac{d^3 y_i}{dt^3} \right|_{t_{n+1}} \frac{h_{n+1}^3}{3!} - \dots \quad i = 1, 2, \dots, N \quad (48)$$

where

$$k_{i,n+1} = y_i(t_{n+1}) - y_i(t_n) \quad (49)$$

$$h_{n+1} = t_{n+1} - t_n \quad (50)$$

Performing an expansion similar to equation (48) for $y_i(t_{n-1})$ about t_{n+1} yields

$$k_{i,n+1} + k_{i,n} = \left. \frac{dy_i}{dt} \right|_{t_{n+1}} (h_{n+1} + h_n) - \left. \frac{d^2 y_i}{dt^2} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n)^2}{2!} + \left. \frac{d^3 y_i}{dt^3} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n)^3}{3!} - \dots \quad (51)$$

The second derivative terms can now be eliminated between equations (48) and (52). Multiplying equation (48) by $(h_{n+1} + h_n)^2 / h_{n+1}^2$ and then subtracting equation (51) gives

$$\frac{(2h_{n+1} + h_n)}{h_{n+1}(h_{n+1} + h_n)} k_{i,n+1} - \frac{h_{n+1}}{(h_{n+1} + h_n)h_n} k_{i,n} = \left. \frac{dy_i}{dt} \right|_{t_{n+1}} - \left. \frac{d^3 y_i}{dt^3} \right|_{t_{n+1}} \frac{h_{n+1}(h_{n+1} + h_n)}{3!} + \dots \quad (52)$$

From the Taylor series expansion by partial derivatives for $(dy_i/dt)_{t_{n+1}}$ about the point t_n we get

$$\left. \frac{dy_i}{dt} \right|_{t_{n+1}} = \left. \frac{dy_i}{dt} \right|_{t_n} + \left. \frac{\partial f_i}{\partial t} \right|_{t_n} h_{n+1} + \sum_{j=1}^N \left. \frac{\partial f_i}{\partial y_j} \right|_{t_n} k_{j,n+1} + \left. \frac{d^3 y_i}{dt^3} \right|_{t_n} \frac{h_{n+1}^2}{2!} + \dots \quad (53)$$

Letting

$$f_{i,n} = \left. \frac{dy_i}{dt} \right|_{t_n} \quad (54)$$

$$\alpha_i(t) = \frac{\partial f_i}{\partial t}, \quad \alpha_{i,n} = \frac{\partial f_i}{\partial t} \Big|_{t_n} \quad (55)$$

$$\beta_{i,j}(t) = \frac{\partial f_i}{\partial y_j}, \quad \beta_{i,j,n} = \frac{\partial f_i}{\partial y_j} \Big|_{t_n} \quad (56)$$

and substituting the last expansion into equation (52) gives

$$\begin{aligned} \frac{(2h_{n+1} + h_n)}{h_{n+1}(h_{n+1} + h_n)} k_{i,n+1} - \frac{h_{n+1}}{(h_{n+1} + h_n)h_n} k_{i,n} = & \left(f_{i,n} + \alpha_{i,n} h_{n+1} + \sum_{j=1}^N \beta_{i,j,n} k_{j,n+1} \right. \\ & \left. + \frac{d^3 y_i}{dt^3} \Big|_{t_n} \frac{h_{n+1}^2}{2!} + \dots \right) - \frac{d^3 y_i}{dt^3} \Big|_{t_{n+1}} \frac{h_{n+1}(h_{n+1} + h_n)}{3!} + \dots \end{aligned} \quad (57)$$

Again, by a Taylor series expansion

$$\frac{d^3 y_i}{dt^3} \Big|_{t_n} \frac{h_{n+1}^2}{2!} = \frac{d^3 y_i}{dt^3} \Big|_{t_{n+1}} \frac{h_{n+1}^2}{2!} + O(h_{n+1}^3) \quad (58)$$

The substitution of equation (58) into equation (57) gives, after combining and rearranging the terms,

$$\begin{aligned} k_{i,n+1} = & \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n} k_{i,n} + \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \left(f_{i,n} + \alpha_{i,n} h_{n+1} + \sum_{j=1}^N \beta_{i,j,n} k_{j,n+1} \right) \\ & + \frac{d^3 y_i}{dt^3} \Big|_{t_{n+1}} \frac{h_{n+1}^2(h_{n+1} + h_n)(2h_{n+1} - h_n)}{3!(2h_{n+1} + h_n)} + O(h_{n+1}^4) \end{aligned} \quad (59)$$

Finally, equation (59) is truncated to produce the implicit equation

$$k_{i,n+1} = \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n} k_{i,n} + \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \left(f_{i,n} + \alpha_{i,n} h_{n+1} + \sum_{j=1}^N \beta_{i,j,n} k_{j,n+1} \right)$$

$$i = 1, 2, \dots, N \quad (60)$$

The solution of the coupled first-order simultaneous differential equations (47) can be obtained by solving at each step the following set of linear equations

$$\left[1 - \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \beta_{i,i,n} \right] k_{i,n+1} - \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \sum_{\substack{j=1 \\ j \neq i}}^N \beta_{i,j,n} k_{j,n+1} = \frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n}$$

$$\times k_{i,n} + \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} (f_{i,n} + \alpha_{i,n} h_{n+1}) \quad i = 1, 2, \dots, N \quad (61)$$

The equations for f_i , α_i , and $\beta_{i,j}$, which are required in order to apply this implicit integration technique to the chemical kinetics problem, are given in appendixes B and C.

Error formula. - The relative error in the numerical solution of $dy_i/dt = f_i$ at the $(n+1)^{st}$ step is defined as

$$E_{i,n+1} = \left| \frac{k_{i,n+1}^{(e)} - k_{i,n+1}}{y_{i,n+1}} \right| \quad (62)$$

where $k_{i,n+1}^{(e)}$ is the exact value of the increment $k_{i,n+1}$. From equation (59),

$$k_{i,n+1}^{(e)} - k_{i,n+1} \approx \frac{d^3 y_i}{dt^3} \bigg|_{t_{n+1}} \frac{h_{n+1}^2 (h_{n+1} + h_n) (2h_{n+1} - h_n)}{3! (2h_{n+1} + h_n)} \quad (63)$$

An expression that can be used to evaluate $\left(d^3 y_i / dt^3\right)_{t_{n+1}}$ will now be obtained. The following equations are the result of Taylor series expansions about the point t_{n+1} :

$$k_{i,n+1} \approx \left. \frac{dy_i}{dt} \right|_{t_{n+1}} h_{n+1} - \left. \frac{d^2 y_i}{dt^2} \right|_{t_{n+1}} \frac{h_{n+1}^2}{2!} + \left. \frac{d^3 y_i}{dt^3} \right|_{t_{n+1}} \frac{h_{n+1}^3}{3!} \quad (64)$$

$$k_{i,n+1} + k_{i,n} \approx \left. \frac{dy_i}{dt} \right|_{t_{n+1}} (h_{n+1} + h_n) - \left. \frac{d^2 y_i}{dt^2} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n)^2}{2!} + \left. \frac{d^3 y_i}{dt^3} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n)^3}{3!} \quad (65)$$

$$k_{i,n+1} + k_{i,n} + k_{i,n-1} \approx \left. \frac{dy_i}{dt} \right|_{t_{n+1}} (h_{n+1} + h_n + h_{n-1}) - \left. \frac{d^2 y_i}{dt^2} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n + h_{n-1})^2}{2!} + \left. \frac{d^3 y_i}{dt^3} \right|_{t_{n+1}} \frac{(h_{n+1} + h_n + h_{n-1})^3}{3!} \quad (66)$$

The preceding set of equations can be solved to give $\left(d^3 y_i / dt^3\right)_{t_{n+1}}$ in terms of $k_{i,n+1}$, $k_{i,n}$, and $k_{i,n-1}$. The solution is

$$\left. \frac{d^3 y_i}{dt^3} \right|_{t_{n+1}} \approx \frac{3!}{(h_{n+1} + h_n + h_{n-1})} \left[\frac{1}{h_{n+1}(h_{n+1} + h_n)} k_{i,n+1} - \frac{(h_{n+1} + 2h_n + h_{n-1})}{(h_{n+1} + h_n)h_n(h_n + h_{n-1})} k_{i,n} + \frac{1}{(h_n + h_{n-1})h_{n-1}} k_{i,n-1} \right] \quad (67)$$

Combining equations (62), (63), and (67) yields

$$E_{i,n+1} = \left[\frac{h_{n+1}^2 (2h_{n+1} - h_n)}{(2h_{n+1} + h_n)(h_{n+1} + h_n + h_{n-1})(h_n + h_{n-1})} \left(\frac{1}{y_{i,n+1}} \right) \right] \\ \times \left[(h_n + h_{n-1}) \frac{k_{i,n+1}}{h_{n+1}} - (h_{n+1} + 2h_n + h_{n-1}) \frac{k_{i,n}}{h_n} + (h_{n+1} + h_n) \frac{k_{i,n-1}}{h_{n-1}} \right] \quad (68)$$

With the definitions

$$C = \frac{(h_{n+1} + h_n)}{(h_n + h_{n-1})} \quad (69)$$

$$D_{i,m} = \frac{k_{i,m}}{h_m} \quad (70)$$

equation (68) can be rewritten as

$$E_{i,n+1} = \left[\frac{h_{n+1}^2 (2h_{n+1} - h_n)}{(2h_{n+1} + h_n)(h_{n+1} + h_n + h_{n-1})} \left(\frac{1}{y_{i,n+1}} \right) \left[(D_{i,n+1} - D_{i,n}) \right. \right. \\ \left. \left. - C(D_{i,n} - D_{i,n-1}) \right] \right] \quad (71)$$

Finally, the relative error in the solution of the set of equations given by equation (47) at the $(n+1)^{\text{st}}$ step is defined to be

$$\epsilon_{n+1} = \max_{i \in I} E_{i,n+1} \quad (72)$$

where I is the set of all dependent variables that are not being omitted from error con-

sideration. The relative error ϵ_{n+1} is used to control both the accuracy and the step size during the numerical integration.

Initial step formula. - The general step formula given by equation (60) requires the value of the increment $k_{i,n}$ and the step size h_n from the previous step. Thus, that formula cannot be used for the initial step. Notice that the error formula (eq. (71)) requires information from two previous steps. We will derive a formula that can be used for the initial two steps to generate initial values for the general step procedure. Let h_1 be the initial step size, t_0 the initial time, and h any second step size. Then equation (60) can be written as

$$y_i(t_0 + h_1 + h) - y_i(t_0 + h_1) = \frac{h^2}{(2h + h_1)} \left[\frac{y_i(t_0 + h_1) - y_i(t_0)}{h_1} \right] + \frac{h(h + h_1)}{(2h + h_1)} \left\{ f_i(t_0 + h_1) \right. \\ \left. + \alpha_i(t_0 + h_1)h + \sum_{j=1}^N \beta_{i,j}(t_0 + h_1) [y_j(t_0 + h_1 + h) - y_j(t_0 + h_1)] \right\} \quad i = 1, 2, \dots, N \quad (73)$$

Taking the limit of equation (73) as h_1 approaches zero, we obtain

$$y_i(t_0 + h) - y_i(t_0) = \frac{h}{2} \frac{dy_i}{dt} \Big|_{t_0} + \frac{h}{2} \left\{ f_i(t_0) + \alpha_i(t_0)h + \sum_{j=1}^N \beta_{i,j}(t_0) [y_j(t_0 + h) - y_j(t_0)] \right\} \quad (74)$$

or more simply,

$$k_{i,1} = f_{i,0}h + \frac{h}{2} \left(\alpha_{i,0}h + \sum_{j=1}^N \beta_{i,j,0} k_{j,1} \right) \quad (75)$$

The initial step is performed by solving the following system of linear equations:

$$\left(1 - \beta_{i,i,0} \frac{h}{2} \right) k_{i,1} - \frac{h}{2} \sum_{\substack{j=1 \\ j \neq i}}^N \beta_{i,j,0} k_{j,1} = h \left(f_{i,0} + \alpha_{i,0} \frac{h}{2} \right) \quad i = 1, 2, \dots, N \quad (76)$$

Since equation (76) requires no information from a previous step, it can be used for each of the initial two steps.

Step-Size Optimization

The numerical integration technique used in the program contains a unique step-size optimization procedure. We define the optimum step size for each integration step to be the largest step size that is consistent with the user's accuracy requirements. The user's accuracy requirements are specified by three input parameters: (1) ϵ_{\max} , the maximum relative error per step, (2) h_{\max} , the maximum step size, and (3) h_{\min} , the minimum step size. The optimum step size, if it exists, must be in the interval (h_{\min}, h_{\max}) and have an associated relative error which does not exceed ϵ_{\max} . In practice, the optimization procedure obtains an approximation of the optimum step size for the given step. The calculation of this approximate optimum step size is based on an empirical method for predicting relative error as a function of step size. The approximation is obtained by performing a limited number of trials to find the largest step size within some subinterval of (h_{\min}, h_{\max}) whose predicted relative error does not exceed ϵ_{\max} . The complete optimization procedure is described in the following paragraphs.

At the conclusion of each step a judgement is made by comparing ϵ_n , the relative error in the step just concluded, with ϵ_{\max} :

- (1) If $\epsilon_n < \frac{1}{2} \epsilon_{\max}$, increase the step size for the $(n+1)^{\text{st}}$ step.
- (2) If $\frac{1}{2} \epsilon_{\max} \leq \epsilon_n \leq \frac{5}{6} \epsilon_{\max}$, use $h_{n+1} = h_n$.
- (3) If $\epsilon_n > \frac{5}{6} \epsilon_{\max}$ and $h_n \geq h_{\min}$, decrease the step size for the $(n+1)^{\text{st}}$ step.
- (4) If $\epsilon_n > \epsilon_{\max}$ and $h_n = h_{\min}$, restart at the n^{th} step.

If the judgement is made to increase the step size for the next step, then a search is made for the optimal h_{n+1} in the interval $[h_n, h_{\max}]$. Analogously, the judgement to decrease the step size for the next step triggers a search for the optimal h_{n+1} in the interval $[h_{\min}, h_n]$. If condition (4) is satisfied then the restart procedure is initiated. The restart procedure consists of repeating the n^{th} step using equation (76) with $h_0 = \frac{1}{2} h_{\min}$ and performing the $(n+1)^{\text{st}}$ step in the same manner. Automatically restarting a case at the beginning of the n^{th} step is exactly the same as manually starting that case with the conditions at the end of the $(n-1)^{\text{st}}$ step as the initial conditions and $\frac{1}{2} h_{\min}$ as the initial step size.

The general step formula equation (60), derived in the previous section is implicit because of the terms $k_{j,n+1}$ on the right side and thus must be solved as a set of simultaneous linear equations. Making the substitution

$$k_{j,n+1} \approx \frac{h_{n+1}}{2} \left(f_{j,n} + \frac{k_{j,n}}{h_n} \right) \quad j \neq i \quad (77)$$

into equation (60) and solving for $k_{i,n+1}$ yields

$$k_{i,n+1} = \left(\frac{h_{n+1}^2}{(2h_{n+1} + h_n)h_n} k_{i,n} + \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \left\{ f_{i,n} + \left[\alpha_{i,n} + \sum_{\substack{j=1 \\ j \neq i}}^N \beta_{i,j,n} \left(\frac{f_{j,n} + k_{j,n}/h_n}{2} \right) \right] h_{n+1} \right\} \right) / \left[1 - \frac{h_{n+1}(h_{n+1} + h_n)}{(2h_{n+1} + h_n)} \beta_{i,i,n} \right] \quad i = 1, 2, \dots, N \quad (78)$$

The set of equations described by (78) is explicit in $k_{i,n+1}$. It requires appreciably fewer operations to obtain values for the increments $k_{i,n+1}$ from (78) than from the simultaneous solution of the equations given by (61). Now, for any given step size h_{n+1} , by using equation (78) as a predictor and equation (60) as a corrector, an approximate solution to the simultaneous equations described by (61) can be obtained. This approximate solution is used to compute a relative error according to the error equations developed in the previous section. The error thus calculated is a prediction of the error that can be expected from the simultaneous solution of equations (61) using the step size h_{n+1} . The step-size optimization is accomplished by searching for a step size h_{n+1} whose predicted error is equal to ϵ_{\max} .

The search technique is a modified form of the conventional half-interval search. Starting with an interval of uncertainty for h_{n+1} of length I (e.g., $I_1 = |h_{\max} - h_{\min}|$), the search successively narrows down the interval until after n iterations ($n \geq 2$), the maximum length of the interval of uncertainty is $I_n = \left(\frac{1}{2}\right)^{n-2} \left(\frac{1}{3} I_1\right)$. The search is terminated when either an h_{n+1} is found whose predicted error is ϵ_{\max} or the limit of 11 on the number of iterations has been reached. In either case the last estimate of h_{n+1} will be used for the next step. Notice that in the worst case $I_{11} \approx 10^{-3} |h_{\max} - h_{\min}|$. Hence, having chosen an input value for h_{\min} on the basis of round-off error and computer time considerations, a reasonable input value for h_{\max} would be $10^3 \cdot h_{\min}$. This would insure that the final interval of uncertainty would be of the order of h_{\min} .

GENERAL DESCRIPTION OF PROGRAM USE

The kinetics program can compute the progress of many different types of static or one-dimensional flow reaction. These include ignition processes, reactions behind a

shock wave, nozzle expansions and assigned pressure reactions. Constant volume and/or constant temperature reactions can also be handled. Computations can be performed for any homogeneous gas mixture containing no more than 25 species. Any species may be considered as long as its thermodynamic data are available in the form described in the section Thermodynamic Data and Species Names. Thirty chemical reactions of the three types already mentioned may be used. There is no limit on the number of each type. For a typical computation the user must provide rate constants and initial values of temperature, pressure, and species concentrations. For a flow reaction, the velocity and an area or pressure profile are also required. Nonzero initial time and position values may be specified. Otherwise, the program sets the starting values of x and t to zero. A detailed description of data card preparation is given in appendix D, and appendix E lists input and selected results for several test cases.

Options

There are several program options that provide for many reaction conditions and these will now be described.

Integration variable. - Either the time or distance version of the basic differential equations may be integrated. The integration variable is chosen by punching the word TIME or DISTANCE on a data card.

Static or flow reaction. - The program was written with flow-kinetic applications in mind. However, static chemical reactions can also be considered very simply by (1) choosing the TIME integration option and (2) setting the flow velocity V equal to zero. The program then integrates equations (3), (17), and (18) for a static system.

Shock wave reactions. - The program contains an option for easily computing the progress of chemical reactions behind a shock wave. When the logical variable SHOCK is set equal to TRUE, the initial conditions are recognized as unshocked gas conditions. The velocity, V is then the shock speed V_s . The program first solves the conservation equations to obtain the conditions of pressure, temperature, and particle velocity behind the shock assuming no reaction. These new conditions and the initial composition are then used to compute the progress of the chemical reactions occurring in the high-temperature region behind the shock wave. The program also computes the final conditions that would exist if these chemical reactions went to complete equilibrium.

Equilibrium calculations. - An option is provided in the program for calculating the final equilibrium conditions for a constant pressure combustion. Both enthalpy and pressure are assumed constant for these calculations, which are triggered by setting the logical variable COMBUS equal to TRUE.

Units options. - The user has a choice of three different systems of units for both

input and output. These are the CGS, U. S. Customary (or FPS), and SI systems. The choice of output units is completely independent of the input units. The exact units used in each system are listed in the sections below on INPUT and OUTPUT.

Assigned profile options. - For any flow-kinetic reaction, an area or pressure profile must be assigned. For a static reaction neither pressure nor area need be assigned. However, a pressure profile may be assigned. The assigned variable may be specified in any of the following ways as a function of time or distance; the choice is independent of the integration variable used:

- (a) A table of assigned variable against distance or time.
- (b) Polynomial coefficients for the equation

$$Q = C_0 + C_1q + C_2q^2 + C_3q^3 \quad (79)$$

where Q is the assigned variable and q is either t or x . Notice that a constant area or pressure profile can be specified by setting $C_3 = C_2 = C_1 = 0$ and C_0 equal to the constant value.

- (c) Special area function. The area may be calculated by the equation

$$A = \frac{1}{1 - \left(\frac{x}{L_m}\right)^\eta} \quad (80)$$

This equation is used to represent laminar and turbulent boundary-layer effects in a shock tube according to the theory of Mirels (refs. 17 to 19). The exponent η must be read into the program. Its value is either 0.5 for a laminar boundary layer or 0.8 for a turbulent boundary layer. The characteristic reaction length parameter, L_m may either be read in or computed by the program. The program uses equation (3) of reference 19 for a laminar boundary layer or equation (4) of reference 18 for a turbulent boundary layer. If L_m is to be computed, three other quantities are read in instead of L_m . These are the shock tube hydraulic diameter D , the unshocked gas viscosity μ , and a boundary-layer thickness parameter β , which can be calculated from equations given in references 18 and 19.

Third-body efficiencies. - The program allows the rate constant for any three-body recombination-dissociation reaction to be adjusted for the efficiencies of different third-body catalysts. The user may read in values of the weighting factor m_{ij} defined in equation (39) for any three-body reaction if the logical variable ALLM1 is set equal to FALSE. All the weighting factors are equal to 1.0 unless changed by the user.

Multiple cases. - Several different cases may be done in one computer run without preparing a complete new data deck for each one. This is done with the use of an ACTION card in each data deck following the first case. The four options that may be used on this ACTION card will be described in a later section.

Constant volume and temperature reactions. - The user has the option of holding either temperature or volume, or both, constant during the chemical reaction computation. The constant temperature condition is obtained by setting the logical variable TCON equal to TRUE. For constant volume the variable RHOCN is set equal to TRUE.

Standard options. - The program has a built-in standard choice for many of the previously mentioned options. None of the given code words or logical variable names has to appear on a data card unless the user wants a nonstandard option. A list of the standard options will be given in a later section.

Thermodynamic Data and Species Names

All thermodynamic data and species names are identical to those used in the chemical equilibrium composition program of Gordon and McBride (ref. 13). Thermodynamic functions are calculated by polynomial equations for C_p , h , S , and G as a function of temperature. The polynomial coefficients were calculated using the thermodynamic properties computer program of McBride and Gordon (ref. 20). The data calculated from these equations are the same as those tabulated in the JANAF thermochemical tables (ref. 21). Seven coefficients A_1, A_2, \dots, A_7 are used for each species in the following equations, where T is the kelvin temperature.

$$\frac{C_p}{R} = A_1 + A_2 T + A_3 T^2 + A_4 T^3 + A_5 T^4 \quad (81)$$

$$\frac{h}{RT} = A_1 + \frac{A_2}{2} T + \frac{A_3}{3} T^2 + \frac{A_4}{4} T^3 + \frac{A_5}{5} T^4 + \frac{A_6}{T} \quad (82)$$

$$\frac{S}{R} = A_1 \ln T + A_2 T + \frac{A_3}{2} T^2 + \frac{A_4}{3} T^3 + \frac{A_5}{4} T^4 + A_7 \quad (83)$$

$$\frac{G}{RT} = A_1 (1 - \ln T) - \frac{A_2}{2} T - \frac{A_3}{6} T^2 - \frac{A_4}{12} T^3 - \frac{A_5}{20} T^4 + \frac{A_6}{T} - A_7 \quad (84)$$

These coefficients A_1, \dots, A_7 are read into the kinetics program either as data cards or card images on magnetic tape. The detailed description of the data cards for each species is given in appendix D. The information on these cards is of three types (1) the species name, (2) the stoichiometric coefficients and element names for each chemical element in the species, and (3) two sets of the thermodynamic coefficients

A_1, A_2, \dots, A_7 for two different temperature ranges. The availability of the thermodynamic data is discussed in appendix F.

Any species can be used in a chemical kinetics computation if its thermodynamic data are read into the computer as indicated and if its name is compiled into the kinetics program in two different routines. The species name, exactly as it is written on the thermodynamic data cards, must first appear in the BLOCK DATA routine. The name array ALSP has space for 75 names containing eight symbols each. As now written, ALSP contains 71 species, so that the user may add only four new species without increasing the dimensions of the array. If this increase in dimensions is not desired, new species may be substituted for any unused ones now in the list. When a species name is

TABLE I. - SPECIES NAMES AND MOLECULAR WEIGHTS INCLUDED IN COMPUTER

PROGRAM "BLOCK DATA" SUBROUTINE

Species	Block data name	Molecular weight	Species	Block data name	Molecular weight	Species	Block data name	Molecular weight
Ar	AR	39.948	CO	CO	28.011	Kr	KR	83.800
B	B	10.811	CO ₂	CO2	44.010	N	N	14.007
BF	BF	29.809	C ₂ F ₂	C2F2	62.019	Ne	NE	20.183
BF ₂	BF2	48.808	C ₂ H	C2H	25.030	NF	NF	33.005
BF ₃	BF3	67.806	C ₂ H ₂	C2H2	26.038	NF ₂	NF2	52.004
BH	BH	11.819	C ₂ H ₄	C2H4	28.054	NF ₃	NF3	71.002
BH ₂	BH2	12.827	C ₂ N	C2N	38.029	NH	NH	15.015
BH ₃	BH3	13.835	Cl	CL	35.453	NH ₂	NH2	16.023
BO	BO	26.810	ClF	CLF	54.451	NH ₃	NH3	17.031
BOF	BOF	45.807	ClF ₃	CLF3	92.448	NO	NO	30.006
BOF ₂	BOF2	64.807	Cl ₂	CL2	70.906	NO+	NO+	30.00555
BO ₂	BO2	42.810	Electron	E	5.48597×10 ⁻⁴	NO ₂	NO2	46.006
B ₂ O ₃	B2O3	69.620	F	F	18.9984	N ₂	N2	28.013
Br	BR	79.909	F ₂	F2	37.997	N ₂ H ₄	N2H4	32.045
Br ₂	BR2	159.82	H	H	1.00797	N ₂ O	N2O	44.012
C	C	12.0112	HCN	HCN	27.026	N ₂ O ₄	N2O4	92.009
CF	CF	31.010	HCl	HCL	36.461	O	O	15.9994
CF ₂	CF2	50.008	HF	HF	20.006	O+	O+	15.99885
CH	CH	13.019	HO ₂	HO2	33.005	O-	O-	15.99995
CH ₂	CH2	14.027	HNO	HNO	31.014	OH	OH	17.007
CH ₂ O ^a	CH2O	30.026	H ₂	H2	2.0159	O ₂	O2	31.997
CH ₃	CH3	15.035	H ₂ O	H2O	18.014	O ₂ ⁻	O2-	31.99935
CH ₄	CH4	16.043	H ₂ O ₂	H2O2	34.014	Xe	XE	131.30
CN	CN	26.018	He	HE	4.0026			

^aFormaldehyde.

listed in ALSP, its molecular weight must be written in the array ALMW in BLOCK DATA. Table I gives a list of the species now recognized by the program and also lists the exact program name and the molecular weight for each species.

A name for each species must also be listed in subroutine INIT. The names are listed in the COMMON block called FAKE and also in NAMELIST START. In this subroutine, species names are used as the FORTRAN concentration variables to simplify the input of initial species concentrations. The name for each species used in INIT is the same as the BLOCK DATA name. In the case of ionic species, a FORTRAN variable name cannot contain special characters, specifically + and -. Therefore, we have adopted the convention of using a P in place of a plus sign and an M in place of a minus sign in INIT. To illustrate this point the table below lists several species from

Species	BLOCK DATA name	Name in COMMON block FAKE and NAMELIST START
H ₂ O	H2O	H2O
B ₂ O ₃	B2O3	B2O3
NO+	NO+	NOP
O+	O+	OP
O-	O-	OM
O ₂ ⁻	O2-	O2M

table I, giving their BLOCK DATA names and their names in subroutine INIT. The exact species name that appears in subroutine INIT must always be used when reading in an initial concentration of any species.

Accuracy Control

Experience has shown that all composition variable errors, $E_{i,n+1}$ need not be considered at every step in calculating ϵ_{n+1} (eq. (72)), the relative error at that step. Quite often, species that have very small concentrations also have large $E_{i,n+1}$ values. If these $E_{i,n+1}$ values are used in the error calculation, the step size will be kept smaller than it has to be. Therefore, some species can usually be eliminated from the error calculation. In this section the methods used to do this are described. In general accuracy and computer running time are controlled by two factors: (1) the assigned

error ϵ_{\max} combined with the species error elimination procedures and (2) the assigned step sizes, especially the initial step size.

Assigned ϵ_{\max} and error elimination. - Two methods of neglecting errors due to trace species are used. The first method is done automatically unless the user wishes to prevent it. Before each new step-size calculation is done, certain species errors are eliminated from consideration in equation (72). The test for elimination is that a species error be equal to at least 15 times the median value of the errors for all the species variables. In the second error omit technique the program is told to neglect

TABLE II. - EFFECT OF ERROR CONTROLS ON HYDROGEN - AIR

IGNITION COMPUTATIONS

(a) Effect of error omit procedures

[Assigned distance, 30 cm.]

Trial	1	2	3	8
Run time, min	22	6	6	8
h_{\max} , cm	0.10	0.10	0.10	0.10
ϵ_{\max}	0.00005	0.00005	0.00005	0.00005
Automatic error elimination	No	Yes	Yes	No
Permanent species error elimination	None	None	H ₂ O ₂	H ₂ O ₂
t, μ sec	162.65	162.65	162.65	162.66
p, atm	1.5166	1.5131	1.5124	1.5116
V, cm/sec	191608	191744	191709	191667
ρ , g/cm ³	1.54257×10^{-4}	1.54155×10^{-4}	1.54184×10^{-4}	1.54216×10^{-4}
T, kelvin	2802	2805	2804	2802
S, cal/gK	2.7451	2.7464	2.7460	2.7454
M	1.7187	1.7184	1.7187	1.7190
γ	1.2518	1.2519	1.2519	1.2518
Mole fractions:				
H ₂	4.387×10^{-2}	4.417×10^{-2}	4.407×10^{-2}	4.396×10^{-2}
OH	2.861×10^{-2}	2.885×10^{-2}	2.877×10^{-2}	2.867×10^{-2}
H ₂ O	0.26282	0.26216	0.26235	0.26262
H	1.674×10^{-2}	1.699×10^{-2}	1.691×10^{-2}	1.680×10^{-2}
O ₂	1.698×10^{-2}	1.708×10^{-2}	1.705×10^{-2}	1.701×10^{-2}
O	6.909×10^{-3}	7.019×10^{-3}	6.984×10^{-3}	6.943×10^{-3}
HO ₂	5.448×10^{-6}	5.503×10^{-6}	5.488×10^{-6}	5.469×10^{-6}
H ₂ O ₂	6.771×10^{-7}	6.817×10^{-7}	6.806×10^{-7}	6.792×10^{-7}
N ₂	0.62407	0.62377	0.62387	0.62398

certain species errors for an entire problem. This is especially needed for a slow reaction such as a long delay ignition. For any ignition reaction the free radical concentrations are usually quite negligible at the start. But, often, the calculated errors for these concentrations are relatively large. If they were used in the step-size calculation, they would keep the step size needlessly small. The permanent error omit procedure must be used for slow reactions, because the automatic method is not sensitive enough to cope with this situation. It has been our experience that the error for any species with a mole fraction of 10^{-4} or less can be neglected with no change in results.

The effect of using the error omit procedure is shown in table II(a), which gives computed results for a hydrogen-air ignition reaction using an IBM 7044-7094 computer. Trial 1 is the standard, in which no species were eliminated from the error analysis. A comparison of trial 2 with trial 1 shows that running time is significantly shortened by using the automatic elimination procedure. The largest change in the results is about a 1-percent change in some of the smaller species mole fractions. Trials 3 and 8 show two things. First, permanently omitting a single species does not reduce running time any further after the automatic omit procedure is used. Second, permanently omitting a single species is not as effective as the automatic procedure in reducing computer time. Computations for other reacting mixtures have shown that the results in table II(a) are quite typical. This is why we have made the automatic error elimination procedure the standard option in the integration routine. However, the user can override these error eliminations by a simple addition to the input data, if any accuracy problem ever occurs. The override should be used if more than three species errors are consistently being neglected.

Table II(b) shows the effect of other factors on accuracy and computer running time. Trial 2 will now be used as the standard of comparison. Trials 2 and 4 show that results are essentially unchanged when ϵ_{\max} , the allowable error, is changed by a factor of 2 from 0.00005 to 0.0001. Trials 4, 6, and 7 show that results are independent of maximum step size as well. Our computations with several reacting mixtures have indicated that $\epsilon_{\max} = 0.0001$ as a maximum relative error gives excellent accuracy with relatively short running times for most situations.

The computing time can, however, be decreased with only a slight loss of accuracy by two different methods. These are (1) increasing ϵ_{\max} and (2) using the permanent error omit procedure for several of the small concentration species. The effect of each of these methods is shown by trials 5 and 9. The ϵ_{\max} value was arbitrarily increased to 0.0003 in trial 5.

When performing computations for very slow reactions the permanent error technique should always be used for all the trace species (mole fraction $\leq 10^{-4}$). For best accuracy the calculation should be stopped when trace species eventually become important. It should then be restarted with these species removed from the permanent omit

TABLE II. - Concluded. EFFECT OF ERROR CONTROLS ON HYDROGEN - AIR IGNITION COMPUTATIONS

(b) Effect of allowed error and permanent error omits using automatic error elimination

[Assigned distance, 30 cm.]

Trial	2	4	6	7	9	5
Run time, min	6	5	5	5	2	3
h_{\max} , cm	0.10	0.10	0.05	0.20	0.10	0.10
ϵ_{\max}	0.00005	0.0001	0.0001	0.0001	0.0001	0.0003
Permanent species error elimination	None	None	None	None	H ₂ O ₂ , HO ₂ H, O, OH	None
t, μ sec	162.65	162.66	162.66	162.65	162.71	162.66
p, atm	1.5131	1.5130	1.5134	1.5145	1.5254	1.5180
V, cm/sec	191744	191724	191715	191797	192204	191968
ρ , g/cm ³	1.54155×10^{-4}	1.54172×10^{-4}	1.54180×10^{-4}	1.54113×10^{-4}	1.53781×10^{-4}	1.53995×10^{-4}
T, kelvin	2805	2805	2805	2808	2828	2815
S, cal/gK	2.7464	2.7463	2.7464	2.7472	2.7539	2.7495
M	1.7184	1.7184	1.7181	1.7178	1.7131	1.7165
γ	1.2519	1.2519	1.2519	1.2519	1.2524	1.2521
Mole fractions:						
H ₂	4.417×10^{-2}	4.415×10^{-2}	4.416×10^{-2}	4.435×10^{-2}	4.583×10^{-2}	4.487×10^{-2}
OH	2.885×10^{-2}	2.882×10^{-2}	2.884×10^{-2}	2.899×10^{-2}	3.020×10^{-2}	2.941×10^{-2}
H ₂ O	0.26216	0.26219	0.26215	0.26171	0.25824	0.26050
H	1.699×10^{-2}	1.697×10^{-2}	1.697×10^{-2}	1.713×10^{-2}	1.836×10^{-2}	1.755×10^{-2}
O ₂	1.708×10^{-2}	1.707×10^{-2}	1.707×10^{-2}	1.714×10^{-2}	1.760×10^{-2}	1.730×10^{-2}
O	7.019×10^{-3}	7.010×10^{-3}	7.013×10^{-3}	7.082×10^{-3}	7.631×10^{-3}	7.271×10^{-3}
HO ₂	5.503×10^{-6}	5.499×10^{-6}	5.498×10^{-6}	5.530×10^{-6}	5.775×10^{-6}	5.616×10^{-6}
H ₂ O ₂	6.817×10^{-7}	6.814×10^{-7}	6.811×10^{-7}	6.837×10^{-7}	7.019×10^{-7}	6.901×10^{-7}
N ₂	0.62377	0.62379	0.62378	0.62359	0.62213	0.62309

list. However, our experience with several chemical systems has shown that acceptable results may often be obtained even when major species are neglected from the error analysis.

The initial step size. - The user specifies a minimum and a maximum step size for any calculation. The program selects h_{\min} as the initial step size unless a different value is given. Using an initial value larger than h_{\min} is another way to decrease computation time. An initial step size even larger than the maximum value may be used when a very slow reaction is being considered. Our experience has shown that the user may choose the largest initial step size that does not cause the integration to break down immediately. Examples of this breakdown are negative species mole fractions and temperatures very different from the starting value. A few trial runs for any new system will show the largest initial step size that may be used.

Input

In this section a general description is given of the several types of data required for a kinetics problem. The exact format of all data cards is given in appendix D.

Chemical reactions and species. - Each chemical reaction is listed on a separate card which has space for two reactant names, two product names, and the three rate constant parameters A_j , n_j , and E_j . The reaction cards may be put in any order, regardless of the type of reaction. The program checks all names on the reaction cards against its species list in the array ALSP. In this way the program automatically builds up the list of species being used in any problem. The availability of rate constant data is discussed in appendix F.

Inert species. - The names of any species present, but not reacting, are listed separately, four per card, following the reaction cards.

Integration variable and units. - A version and units card follows the inert species list. It contains the code words for the integration variable (DISTANCE or TIME) and for the assigned variable (AREA or PRESSURE). It also contains the codes for input and output units (CGS, FPS, or SI). Table III gives the units needed with each of these three options for the input data.

TABLE III. - INPUT UNITS FOR THREE UNITS SYSTEMS

Variable	Internal (CGS)	FPS	SI
Velocity	cm/sec	ft/sec	m/sec
Temperature	K	$^{\circ}\text{R}$	K
Density	g/cm ³	lbm/ft ³	kg/m ³
Pressure ^a	atm	lbf/ft ²	N/m ²
Length	cm	ft	m
Area	cm ²	ft ²	m ²
Species concentration	Mole fraction or mass fraction	Mole fraction or mass fraction	Mole fraction or mass fraction

^aPressure may also be specified as mmHg (torr) in all systems.

Problem data. - Most of the input data for a problem are listed in a NAMELIST called PROB, which follows the version card. PROB contains the assigned variable profile information, printout information, and the integration controls. It also contains the logical variables SHOCK, COMBUS, ALLM1, TCON, and RHOCN.

Efficiencies for three-body recombination-dissociation reactions. - The third-body catalyst efficiencies m_{ij} are contained on one or more cards following NAMELIST

PROB. These cards are permitted only if ALLM1 has been set equal to FALSE. Each card contains up to three species names with corresponding m_{ij} values for a single reaction. The reaction is written on each of these cards exactly as it appears on the reaction card.

Starting conditions. - The starting values for the fluid dynamic variables and the composition of the reacting gas are listed in a NAMELIST called START, which follows either the third-body efficiency cards or NAMELIST PROB. In general, five variables make up the initial conditions in addition to the species starting concentrations. The program initializes all of these to zero. These variables, therefore, do not have to actually appear in NAMELIST START unless their values are nonzero. Four of these initial values are always x , t , T , and either V or Mach number. For the last fluid-dynamic variable the user has a choice of either p , ρ , A , or mass flow rate \dot{m} . The choice is determined by the profile that has been assigned in NAMELIST PROB. For an assigned area problem one may list either p , ρ , or \dot{m} . For an assigned pressure problem either A or \dot{m} may be used.

Species starting concentrations can be given either as mole fractions or mass fractions. The program name of the species is used as its concentration variable name. For example, $H_2 = 0.50$ means that the concentration of H_2 is 0.5 in the mixture. The program interprets these concentration numbers as mole fractions unless it is told that they are mass fractions. This is done by setting the variable MOLEF equal to FALSE.

Species omitted from error calculations. - It was mentioned earlier that the program can be made to neglect minor species errors during its step-size calculation for a complete case. These "permanently omitted" species are listed, four per card, immediately following NAMELIST START.

Output

The program has both standard and optional output. The exact output units used for each of the three systems, CGS, FPS, and SI, are listed in table IV. All computed results are completely independent of the print station positions. A special step is made to each print station and the independent variable is then reset to its previous value. From this point it is increased by the normally calculated step size to a value greater than the print station value.

Standard output. - The following data will be listed if no special codes are used in the input data:

- (1) Reaction time¹
- (2) Axial position and flow cross-section area

¹Gas particle time for a shock wave reaction.

TABLE IV. - OUTPUT UNITS FOR THREE UNITS SYSTEMS

Variable	Internal (CGS) units	FPS units	SI units
Velocity	cm/sec	ft/sec	m/sec
Temperature	K	^o R	K
Density	g/cm ³	lbm/ft ³	kg/m ³
Pressure	atm	lbf/ft ²	N/m ²
Time	sec	sec	sec
Length	cm	ft	m
Area	cm ²	ft ²	m ²
Species concentration	Mole fraction, mass fraction, (g/mole) /cm ³	Mole fraction, mass fraction, (lb mole) /ft ³	Mole fraction, mass fraction, (kg mole) /m ³
Species production rate	(g-mole)/cm ³ sec	(lb mole)/ft ³ sec	(kg mole)/m ³ sec
Net reaction conversion rate	$\frac{\text{g-mole}}{\text{cm}^3 \text{ sec}} / \rho^2$	$\frac{\text{lb-mole}}{\text{ft}^3 \text{ sec}} / \rho^2$	$\frac{\text{kg mole}}{\text{m}^3 \text{ sec}} / \rho^2$
Net energy exchange rate	$\frac{\text{cal}}{\text{cm}^3 \text{ sec}} / \rho^2$	$\frac{\text{Btu}}{\text{ft}^3 \text{ sec}} / \rho^2$	$\frac{\text{J}}{\text{m}^3 \text{ sec}} / \rho^2$
Reaction rate constant	cgs units ^a	cgs units ^a	cgs units ^a
dV/d q	(cm/sec)/unit q	(cm/sec)/unit q	(cm/sec)/unit q
dρ/d q	(g/cm ³)/unit q	(g/cm ³)/unit q	(g/cm ³)/unit q
dT/d q	K/unit q	K/unit q	K/unit q
dσ _i /d q	(g-mole/g)/unit q	(g-mole/g)/unit q	(g-mole/g)/unit q
Mass flow rate	g/sec	lbm/sec	kg/sec
Entropy	cal/g K	Btu/lb ^o R	J/kg K

^aSee table V.

- (3) Pressure, velocity, density, and temperature of the gas mixture
- (4) Entropy per unit mass and frozen heat capacity ratio for the gas mixture. The entropy S is computed from

$$S = R \sum_{i=1}^N \sigma_i \left[\frac{S_i}{R} - \ln \sigma_i - \ln(pM_w) \right] \quad (85)$$

- (5) Local Mach number
- (6) Mole fraction of each species in the gas mixture
- (7) Molar concentration of each mixture species
- (8) Net species production rate W_i defined by equation (31) (This is the net rate of change of each molar concentration due to all chemical reactions.)
- (9) Net reaction conversion rate, X_j , defined by equations (36), (37), (40), (41), or (42) for the three types of chemical reactions being considered
- (10) Rate constant value, k_j for each reaction (This is just the value given by equation (33). For a dissociation or recombination reaction, the third-body efficiency is assumed to be 1.0.)
- (11) Mixture molecular weight
- (12) Mass fraction sum
- (13) Total energy exchange rate defined by

$$X_H = \sum_{j=1}^l X_{H,j} \quad (86)$$

where l is the number of reactions and $X_{H,j}$ is defined in equation (43) (The quantity X_H is proportional to the net heat release rate for the entire complex reaction and may be useful in ignition reactions.)

- (14) Derivatives of all dependent integration variables, V , T , ρ , and each σ_i , with respect to the independent variable
- (15) Increments and relative errors - the computed increments $k_{i,n+1}$ and relative errors $E_{i,n+1}$ as defined in equations (49) and (62) for the current integration step
- (16) Integration indicators
 - (a) Steps from last print
 - (b) Average step size since last print
 - (c) Controlling variable - the variable with the largest error $E_{i,n+1}$
 - (d) Relative error - the value of ϵ_{n+1} for the step being printed out
 - (e) Any species that will be automatically eliminated from error consideration for the next step

Optional output. - Several changes and additions to the standard output may be made:

- (1) Species mass fraction may be listed in place of molar concentration by setting the logical variable CONC equal to FALSE in NAMELIST PROB.
- (2) Net energy exchange rate for each reaction $X_{H,j}$ defined by equation (43) may be listed in place of net reaction conversion rate by setting the logical variable EXCHR equal to TRUE in NAMELIST PROB.

(3) The program has an option for listing certain additional data or intermediate output at each print station. These data are useful either for studying the effect of each individual reaction on gas composition or for diagnosing any program problems. This option is chosen by setting the variable DBUGO equal to TRUE in NAMELIST PROB. The following quantities are then listed:

- (a) The molar rate of production of species i due to reaction j , ω_{ij} , defined by equation (35)
- (b) The quantities \mathcal{A} and \mathcal{B} or \mathcal{A}^* and \mathcal{B}^*
- (c) If area has been assigned, the quantities dA/dq , d^2A/dq^2 and either

$$\left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right)$$

or

$$\left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A}^* \right)$$

If pressure has been assigned, the quantities dp/dq , d^2p/dq^2 and $(1/p)(dp/dq)$ are printed out. Here q is the independent variable, either t or x .

PROGRAM ORGANIZATION

The program is organized into the following five sections: (1) control, (2) input/output, (3) shock/combustion, (4) chemical kinetics, and (5) numerical integration. An effort was made in writing the program to make each of the last three sections self-contained except for the reading and processing of input data. The shock/combustion section uses subroutine THRM from the chemical kinetics section, but is independent in all other respects. The chemical kinetics and numerical integration sections are complete in themselves. The next sections describe the function of each program section and of each subroutine in the section. The names of nonstandard entry points into a subroutine are given in parentheses following the subroutine name. Flow charts for key subroutines (figs. 1 to 6) are found in appendix G along with the FORTRAN listing.

Control Section

The control section is synonymous with the main program GCKP. It provides for

problem setup through a series of subroutine calls. It also monitors the numerical integration and provides an output call whenever a print station is reached (see fig. 1).

Input/Output Section

This section provides for the reading, converting and writing of all input data and kinetics results. It also performs all the necessary bookkeeping functions such as building tables, setting option switches, and storing data for later use.

KINP (RINP). - Provides for the processing of all input data. It initializes, sets all standard options, reads input data and converts it to internal (CGS) units, calculates reference conditions, builds tables and provides calls for shock and combustion calculations (see fig. 2).

CIMAGE. - Prints a card image of each data card.

NAMBLK. - Contains, in block data format, logical tape unit numbers and alphanumeric data for testing and output.

BLCK. - Contains, in block data format, the master species list and the molecular weight of each species in that list.

INIT. - Reads the initial conditions by means of NAMELIST START and stores initial species concentrations using a table provided by KINP.

OUTP (OUT1, OUT2, OUT3). - Provides all output except shock and combustion results. It converts output data from internal units to user's requested output units and calculates parameters which are required only as output such as total entropy and net energy exchange rates.

Shock/Combustion Section

The frozen and equilibrium shock and the equilibrium combustion calculations are performed in this section. It converts and writes its own output and provides for the transfer of frozen shock results to the input/output section as initial conditions for the kinetics calculations. Except for reading input and calculating thermodynamic properties, this section is independent of the other sections.

COMB. - Provides the necessary setup and subroutine calls for the calculation of a constant pressure equilibrium combustion.

SHOK. - Provides the necessary setup and subroutine calls for the calculation of both an equilibrium and a frozen shock.

SHOCKS. - Solves the shock equations for both the equilibrium and frozen cases.

ELEMNT. - Collects chemical element data for equilibrium calculations. These

data include a list of the elements present and the concentration of each of these elements in atoms per gram.

EQLBRM. - This routine, and the following two, are modified versions of routines used in the chemical equilibrium composition program described in reference 13. It calculates equilibrium composition and properties for an assigned set of conditions - assigned temperature and pressure for a shock, assigned enthalpy and pressure for a combustion.

MATRIX. - Used by subroutine EQLBRM to construct matrices required in equilibrium calculations.

GAUSS. - Solves the linear equations which are set up by subroutine MATRIX.

SPOUT (ECOUT, ESOUT, FSOUT). - Provides for the output of all shock and combustion results. It converts output data to the user's requested output units, transfers frozen shock results to the input/output section and calculates the characteristic shock tube reaction length L_m in centimeters if this calculation is required.

Chemical Kinetics Section

The calculation of all chemical and flow parameters is performed in this section. In particular, thermodynamic functions are evaluated, reaction and species production rates are computed, and all required partial and total derivatives are calculated. This section is independent of all but the input/output section.

PRED (PRED1). - Performs all necessary prederivative calculations. This routine calls for or computes directly the thermodynamic properties, reaction rates, equilibrium constants, pressure, specific heat ratio and Mach number as well as other parameters required for the calculation of derivatives (see fig. 3).

DERV. - Calculates all partial and total derivatives with respect to the variable of integration (see fig. 4).

PARD. - Calculates all partial derivatives with respect to the chemical and flow variables (see fig. 5).

THRM. - Computes the (dimensionless) thermodynamic properties h_i/RT , G_i/RT , S_i/R , $(C_p)_i/R$, and $(dC_p/dT)_i/R$ from polynomial curve fits (see ref. 20).

CUBS (CINP). - Provides for the calculation of the assigned variable and its derivatives. If the assigned variable is specified by a table, then the variable and its derivatives are computed by cubic spline interpolation.

Numerical Integration Section

This section sets up and solves the implicit equations, computes the relative error,

and performs the step-size optimization at each step. It contains the automatic species elimination calculations for omitting from error considerations those species with non-representative errors. This section of the program is independent of the other sections.

INTE (INTI, INTC, INTG). - Provides control of the numerical integration procedure during each step. It calls for the implicit equations to be set up and solved, checks for restart conditions, and calls for the step-size optimization (see fig. 6).

CASM (CASI, CASG). - Sets up the implicit equations as an augmented matrix, calls for the solution, and updates all the dependent variables after the increments have been calculated.

LESV. - Solves the implicit equations for the increments $k_{i,n+1}$ using the matrix provided by subroutine CASM.

ERROR. - Computes the relative error and determines the controlling variable at each step.

PERR. - Provides an approximate error for any assigned step size by obtaining an approximate solution of the implicit equations. This routine is used in the step-size optimization procedure to predict the error which can be expected from any given step size.

AUTO. - Provides for the automatic elimination from error considerations of species with nonrepresentative errors. A species error E_i is considered to be non-representative if $E_i > 15 \cdot E_m$ where E_m is the median of the errors associated with those species which have not been permanently neglected from all error considerations.

SEARCH. - A sequential direct search routine which is used in the step-size optimization procedure.

CONCLUDING REMARKS

A general chemical kinetics computer program has been described for calculating the history of many different complex gas-phase reactions. Its main features are flexibility, ease of use and efficiency of computation for both slow and very fast reactions. The species and reactions to be considered are specified by the user. The program is especially useful for ignition and combustion reactions and complex reactions behind a shockwave. In addition it may be used for many types of homogeneous reaction in either a static system or one-dimensional flow. Further information on availability of the program may be obtained from the authors.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, August 26, 1971,
129-01.

APPENDIX A

SOLUTION OF SHOCK WAVE EQUATIONS

The shock equations (eqs. (44) to (46)), are solved by an iterative method. For both frozen and equilibrium conditions, one makes estimates of the final temperature and pressure p_f and T_f . Then a Newton-Raphson method is used to calculate corrections to these estimates and converge on the correct values. The shock equations are transformed and combined for this solution. First, equation (44) gives

$$V^2 = \left(\frac{\rho_1}{\rho} \right)^2 V_s^2 \quad (A1)$$

This equation is used in equations (45) and (46) to eliminate V and gives, after some rearrangement

$$\left[1 - \left(\frac{\rho_1 V_s^2}{p_1} \right) \left(\frac{\rho_1}{\rho} - 1 \right) \right] - \frac{p}{p_1} = 0 \quad (A2)$$

$$\left[h_1 + \frac{V_s^2}{2} - \frac{V_s^2}{2} \left(\frac{\rho_1}{\rho} \right)^2 \right] - h = 0 \quad (A3)$$

Using the equation of state (eq. (8)) for no change in gas composition gives

$$\frac{\rho_1}{\rho} = \left(\frac{p_1}{p} \right) \left(\frac{T}{T_1} \right) = \frac{\mathcal{T}}{P} \quad (A4)$$

where we have defined the new variables $\mathcal{T} = T/T_1$ and $P = p/p_1$.

Equations (A2) and (A3) can now be written as functions of the pressure and temperature ratios across the shock:

$$\left[1 - \left(\frac{\rho_1 V_s^2}{p_1} \right) \left(\frac{\mathcal{T}}{P} - 1 \right) \right] - P = 0 \quad (\text{A5})$$

$$\left[h_1 + \frac{V_s^2}{2} - \frac{V_s^2}{2} \left(\frac{\mathcal{T}}{P} \right)^2 \right] - h = 0 \quad (\text{A6})$$

These equations are solved iteratively for the final ratios \mathcal{T}_f and P_f across the shock. First estimates of \mathcal{T} and P are obtained from the following equations:

$$P_0 = \frac{2\gamma M_s^2 - \gamma + 1}{\gamma + 1} \quad (\text{A7})$$

$$\mathcal{T}_0 = \frac{P_0 \left(\frac{2}{M_s^2} + \gamma - 1 \right)}{\gamma + 1} \quad (\text{A8})$$

These are the exact solutions of equations (44) to (46) when heat capacity is assumed to be independent of temperature. Then the Newton-Raphson procedure is used to calculate corrections to $\ln P$ and $\ln \mathcal{T}$, where it is assumed that

$$\ln P_{n+1} = \ln P_n + \Delta \ln P \quad (\text{A9})$$

$$\ln \mathcal{T}_{n+1} = \ln \mathcal{T}_n + \Delta \ln \mathcal{T} \quad (\text{A10})$$

where n indicates the n^{th} iteration step. Logarithmic differentiation is used to obtain rapid convergence of the procedure. We define the quantities

$$p^* = 1 - \left(\frac{\rho_1 V_s^2}{p_1} \right) \left(\frac{\mathcal{T}}{P} - 1 \right) \quad (\text{A11})$$

$$h^* = h_1 + \frac{V_s^2}{2} - \frac{V_s^2}{2} \left(\frac{\mathcal{T}}{P} \right)^2 \quad (\text{A12})$$

Then equations (A5) and (A6) can be written as

$$F(\mathcal{T}, P) = p^* - P = 0 \quad (\text{A13})$$

$$G(\mathcal{T}, P) = h^* - h = 0 \quad (\text{A14})$$

Substituting equations (A9) and (A10) and using logarithmic differentiation gives the following pair of linear equations for the corrections $\Delta \ln P$ and $\Delta \ln \mathcal{T}$ in the Newton-Raphson method:

$$\left(\frac{\partial F}{\partial \ln \mathcal{T}} \right)_n \Delta \ln \mathcal{T} + \left(\frac{\partial F}{\partial \ln P} \right)_n \Delta \ln P = -F_n \quad (\text{A15})$$

$$\left(\frac{\partial G}{\partial \ln \mathcal{T}} \right)_n \Delta \ln \mathcal{T} + \left(\frac{\partial G}{\partial \ln P} \right)_n \Delta \ln P = G_n \quad (\text{A16})$$

In these equations subscript n indicates evaluation of either the function or its derivative for the estimated values P_n and \mathcal{T}_n . This method of solution is the one used by Gordon and McBride (ref. 13). This procedure is used for both the equilibrium and the frozen shock conditions. The only difference in method for the two situations is the way the enthalpy is computed for the shocked gas. For the frozen shock conditions, h is calculated at the estimated temperature T for the original gas composition. In the equilibrium case the shocked gas enthalpy depends on T and also the changing gas composition due to reaction. Therefore, the estimated T and p are first used to perform an equilibrium chemical reaction calculation. This gives the estimated final composition of the shocked gas. This composition and the estimated T are then used to calculate the enthalpy h used in equation (A14) to compute the function $G(\mathcal{T}, P)$ in the Newton-Raphson method.

APPENDIX B

CALCULATION OF PARTIAL DERIVATIVES FOR THE IMPLICIT INTEGRATION PROCEDURE

Several partial derivatives must be calculated for solving the system

$$\frac{dy_i}{dq} = f_i(q, y_1, y_2, \dots, y_m) \quad (B1)$$

where

$$q = t \text{ or } x \quad i = 1, 2, \dots, m$$

The necessary derivatives are

$$\alpha_i = \frac{\partial f_i}{\partial q} \quad i = 1, 2, \dots, m \quad (B2)$$

$$\beta_{i,j} = \frac{\partial f_i}{\partial y_j} \quad i, j = 1, 2, \dots, m \quad (B3)$$

For this program the following identifications are made for the y_i 's:

$$y_1 = V$$

$$y_2 = \rho$$

$$y_3 = T$$

$$y_{i+3} = \sigma_i \quad i = 1, 2, \dots, N$$

where N is the number of species in the gas.

Derivatives must be calculated for two different equation systems: either equations (3) and (9) to (11) for assigned area or equations (3) and (25) to (27) for assigned pres-

sure. For convenience in the calculations simplified notation will be used to represent the several derivatives of the y_i 's.

$$f_1 = \frac{dV}{dq}$$

$$f_2 = \frac{d\rho}{dq}$$

$$f_3 = \frac{dT}{dq}$$

$$f_{i+3} = \frac{d\sigma_i}{dq} \quad i = 1, 2, \dots, N$$

In the following equations the symbols \mathcal{A}^* and \mathcal{B}^* will not be used. The symbols \mathcal{A} and \mathcal{B} are assumed to have definitions consistent with the particular f_i definitions being used. (See eqs. (12), (13), (23), and (24).)

Assigned Area Equations

From equations (3) and (9) to (11) the following equations are used for the f_i 's:

$$f_1 = \frac{V}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \quad (B4)$$

$$f_2 = -\rho \left[\frac{M^2}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) + \mathcal{A} \right] \quad (B5)$$

$$f_3 = -T \left[\frac{(\gamma - 1)M^2}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) + \mathcal{B} \right] \quad (B6)$$

$$f_{i+3} = \frac{W_i}{r} \quad i = 1, 2, \dots, N \quad (B7)$$

where

$$r = \rho \text{ for } q = t$$

$$= \rho V \text{ for } q = x$$

The α_i 's are most easily obtained because only one quantity, the area A is an explicit function of q . The results are

$$\alpha_1 = \frac{\partial f_1}{\partial q} = \frac{V}{A(M^2 - 1)} \left[\frac{d^2 A}{dq^2} - \frac{1}{A} \left(\frac{dA}{dq} \right)^2 \right] \quad (B8)$$

$$\alpha_2 = \frac{\partial f_2}{\partial q} = -\frac{\rho M^2}{A(M^2 - 1)} \left[\frac{d^2 A}{dq^2} - \frac{1}{A} \left(\frac{dA}{dq} \right)^2 \right] \quad (B9)$$

$$\alpha_3 = \frac{\partial f_3}{\partial q} = -\frac{T(\gamma - 1)M^2}{A(M^2 - 1)} \left[\frac{d^2 A}{dq^2} - \frac{1}{A} \left(\frac{dA}{dq} \right)^2 \right] \quad (B10)$$

$$\alpha_{i+3} = \frac{\partial f_{i+3}}{\partial q} = 0 \quad i = 1, 2, \dots, N \quad (B11)$$

The assigned area can be read in as a function of x when t is the integration variable, and vice-versa. Therefore, the following transformations may be required:

$$\frac{dA}{dt} = V \frac{dA}{dx} \quad (B12)$$

$$\frac{d^2 A}{dt^2} = V^2 \frac{d^2 A}{dx^2} + f_1 \frac{dA}{dx} \quad (B13)$$

or

$$\frac{dA}{dx} = \frac{1}{V} \frac{dA}{dt} \quad (B14)$$

$$\frac{d^2 A}{dx^2} = \frac{1}{V^2} \left(\frac{d^2 A}{dt^2} - f_1 \frac{dA}{dt} \right) \quad (B15)$$

The $\beta_{1,j}$'s are obtained by differentiating equation (B4). The additional partial derivatives which appear in the following equations are evaluated in appendix C.

$$\beta_{1,1} = \frac{\partial f_1}{\partial V} = \frac{1}{(M^2 - 1)} \left[\left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) - f_1 \frac{\partial M^2}{\partial V} - V \frac{\partial \mathcal{A}}{\partial V} \right] \quad (B16)$$

$$\beta_{1,2} = \frac{\partial f_1}{\partial \rho} = - \frac{V}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \rho} \quad (B17)$$

$$\beta_{1,3} = \frac{\partial f_1}{\partial T} = - \frac{V}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial T} - \frac{f_1}{(M^2 - 1)} \frac{\partial M^2}{\partial T} \quad (B18)$$

$$\beta_{1,j+3} = \frac{\partial f_1}{\partial \sigma_j} = - \frac{1}{(M^2 - 1)} \left(V \frac{\partial \mathcal{A}}{\partial \sigma_j} + f_1 \frac{\partial M^2}{\partial \sigma_j} \right) \quad j = 1, 2, \dots, N \quad (B19)$$

The $\beta_{2,j}$'s are obtained from equation (B5)

$$\beta_{2,1} = \frac{\partial f_2}{\partial V} = \frac{\rho}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial V} + \frac{\rho}{(M^2 - 1)^2} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \frac{\partial M^2}{\partial V} \quad (B20)$$

$$\beta_{2,2} = \frac{\partial f_2}{\partial \rho} = \frac{\rho}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \rho} + \frac{f_2}{\rho} \quad (B21)$$

$$\beta_{2,3} = \frac{\partial f_2}{\partial T} = \frac{\rho}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial T} + \frac{\rho}{(M^2 - 1)^2} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \frac{\partial M^2}{\partial T} \quad (B22)$$

$$\beta_{2,j+3} = \frac{\partial f_2}{\partial \sigma_j} = \frac{\rho}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \sigma_j} + \frac{\rho}{(M^2 - 1)^2} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \frac{\partial M^2}{\partial \sigma_j} \quad j = 1, 2, \dots, N \quad (B23)$$

The $\beta_{3,j}$'s are obtained from equation (B6)

$$\beta_{3,1} = \frac{\partial f_3}{\partial V} = T \left[\frac{(\gamma - 1)M^2}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial V} + \frac{(\gamma - 1)}{(M^2 - 1)^2} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \frac{\partial M^2}{\partial V} - \frac{\partial \mathcal{B}}{\partial V} \right] \quad (B24)$$

$$\beta_{3,2} = \frac{\partial f_3}{\partial \rho} = T \left[\frac{(\gamma - 1)M^2}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \rho} - \frac{\partial \mathcal{B}}{\partial \rho} \right] \quad (B25)$$

$$\begin{aligned} \beta_{3,3} = \frac{\partial f_3}{\partial T} = & \frac{(\gamma - 1)M^2 T}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial T} + \frac{(\gamma - 1)T}{(M^2 - 1)^2} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \frac{\partial M^2}{\partial T} \\ & - \frac{M^2 T}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \frac{\partial \gamma}{\partial T} - T \frac{\partial \mathcal{B}}{\partial T} + \frac{f_3}{T} \end{aligned} \quad (B26)$$

$$\begin{aligned} \beta_{3,j+3} = \frac{\partial f_3}{\partial \sigma_j} = & T \left[\frac{(\gamma - 1)M^2}{(M^2 - 1)} \frac{\partial \mathcal{A}}{\partial \sigma_j} + \frac{(\gamma - 1)}{(M^2 - 1)^2} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \frac{\partial M^2}{\partial \sigma_j} \right. \\ & \left. - \frac{M^2}{(M^2 - 1)} \left(\frac{1}{A} \frac{dA}{dq} - \mathcal{A} \right) \frac{\partial \gamma}{\partial \sigma_j} - \frac{\partial \mathcal{B}}{\partial \sigma_j} \right] \quad j = 1, 2, \dots, N \end{aligned} \quad (B27)$$

To obtain $\beta_{i+3,j}$ equation (B7) is rewritten using equations (31) and (35) to obtain (using subscript s to indicate the chemical reactions)

$$f_{i+3} = \frac{\rho^2}{r} \sum_{s=1}^l (\nu'_{i,s} - \nu_{i,s}) X_s \quad i = 1, 2, \dots, N \quad (B28)$$

Taking derivatives of equation (B28) gives

$$\beta_{i+3,1} = \frac{\partial f_{i+3}}{\partial V} = 0 \quad i = 1, 2, \dots, N \quad (\text{B29})$$

$$\beta_{i+3,2} = \frac{\partial f_{i+3}}{\partial \rho} = \frac{f_{i+3}}{\rho} + \frac{\rho^2}{r} \sum_{s=1}^l (\nu'_{i,s} - \nu_{i,s}) \frac{\partial X_s}{\partial \rho} \quad i = 1, 2, \dots, N \quad (\text{B30})$$

$$\beta_{i+3,3} = \frac{\partial f_{i+3}}{\partial T} = \frac{\rho^2}{r} \sum_{s=1}^l (\nu'_{i,s} - \nu_{i,s}) \frac{\partial X_s}{\partial T} \quad i = 1, 2, \dots, N \quad (\text{B31})$$

$$\beta_{i+3,j+3} = \frac{\partial f_{i+3}}{\partial \sigma_j} = \frac{\rho^2}{r} \sum_{s=1}^l (\nu'_{i,s} - \nu_{i,s}) \frac{\partial X_s}{\partial \sigma_j} \quad i = 1, 2, \dots, N \quad j = 1, 2, \dots, N \quad (\text{B32})$$

Assigned Pressure Equations

From the system of equations (3) and (25) to (27) the following equations are now used for the f_i 's:

$$f_1 = -\frac{1}{\rho V} \frac{dp}{dq} \quad (\text{B33})$$

$$f_2 = \rho \left(\frac{1}{\gamma p} \frac{dp}{dq} - \mathcal{A} \right) \quad (\text{B34})$$

$$f_3 = T \left[\left(\frac{\gamma - 1}{\gamma} \right) \frac{1}{p} \frac{dp}{dq} - \mathcal{B} \right] \quad (\text{B35})$$

For f_{i+3} , $i = 1, 2, \dots, N$, the equations are identical to those for the assigned area system (eq. (B7)). This means that equations for α_{i+3} , $\beta_{i+3,1}$, $\beta_{i+3,2}$, $\beta_{i+3,3}$, and

$\beta_{i+3,j+3}$ need not be derived again in the assigned pressure system for i and $j = 1, 2, \dots, N$. They are identical to equations (B29) to (B32). The equations for the rest of the α_i 's and $\beta_{i,j}$'s are as follows:

$$\alpha_1 = -\frac{1}{\rho V} \frac{d^2 p}{dq^2} \quad (B36)$$

$$\alpha_2 = \frac{\rho}{\gamma p} \left[\frac{d^2 p}{dq^2} - \frac{1}{p} \left(\frac{dp}{dq} \right)^2 \right] \quad (B37)$$

$$\alpha_3 = \frac{T}{p} \left(\frac{\gamma - 1}{\gamma} \right) \left[\frac{d^2 p}{dq^2} - \frac{1}{p} \left(\frac{dp}{dq} \right)^2 \right] \quad (B38)$$

If pressure derivative transformations between x and t are required, they are identical in form to equations (B12) to (B15).

$$\beta_{1,1} = -\frac{f_1}{V} \quad (B39)$$

$$\beta_{1,2} = -\frac{f_1}{\rho} \quad (B40)$$

$$\beta_{1,3} = 0 \quad (B41)$$

$$\beta_{1,j+3} = 0 \quad j = 1, 2, \dots, N \quad (B42)$$

$$\beta_{2,1} = -\rho \frac{\partial \mathcal{A}}{\partial V} \quad (B43)$$

$$\beta_{2,2} = \frac{f_2}{\rho} - \rho \frac{\partial \mathcal{A}}{\partial \rho} \quad (B44)$$

$$\beta_{2,3} = -\rho \frac{\partial \mathcal{A}}{\partial T} - \frac{\rho}{p\gamma^2} \frac{dp}{dq} \frac{\partial \gamma}{\partial T} \quad (B45)$$

$$\beta_{2,j+3} = -\rho \frac{\partial \mathcal{A}}{\partial \sigma_j} - \frac{\rho}{\gamma^2 p} \frac{dp}{dq} \frac{\partial \gamma}{\partial \sigma_j} \quad j = 1, 2, \dots, N \quad (\text{B46})$$

$$\beta_{3,1} = -T \frac{\partial \mathcal{B}}{\partial V} \quad (\text{B47})$$

$$\beta_{3,2} = -T \frac{\partial \mathcal{B}}{\partial \rho} \quad (\text{B48})$$

$$\beta_{3,3} = \frac{f_3}{T} + \mathcal{B} - T \frac{\partial \mathcal{B}}{\partial T} + \frac{T}{p\gamma^2} \frac{dp}{dq} \frac{\partial \gamma}{\partial T} \quad (\text{B49})$$

$$\beta_{3,j+3} = \frac{T}{p\gamma^2} \frac{dp}{dq} \frac{\partial \gamma}{\partial \sigma_j} - T \frac{\partial \mathcal{B}}{\partial \sigma_j} \quad j = 1, 2, \dots, N \quad (\text{B50})$$

APPENDIX C

ADDITIONAL PARTIAL DERIVATIVES

The equations for the $\beta_{i,j}$ partial derivatives in appendix B require additional derivatives for their evaluation. These are the partial derivatives of M^2 , γ , \mathcal{A} , \mathcal{B} , and the X_s 's with respect to V , ρ , T , and the σ_i 's.

Derivatives of M^2

The following relations are readily obtained from equation (14)

$$\frac{\partial M^2}{\partial \sigma_i} = -M^2 M_w - \frac{M^2}{\gamma} \frac{\partial \gamma}{\partial \sigma_i} \quad (C1)$$

$$\frac{\partial M^2}{\partial V} = \frac{2VM_w}{\gamma RT} \quad (C2)$$

$$\frac{\partial M^2}{\partial T} = -\frac{M^2}{T} - \frac{M^2}{\gamma} \frac{\partial \gamma}{\partial T} \quad (C3)$$

Derivatives of γ

The following derivatives are obtained from equation (15)

$$\frac{\partial \gamma}{\partial \sigma_i} = \gamma(\gamma - 1) \left[M_w - \frac{(C_p)_i}{C_p} \right] \quad (C4)$$

$$\frac{\partial \gamma}{\partial T} = -\frac{\gamma(\gamma - 1)}{C_p} \sum_{i=1}^N \sigma_i \frac{d(C_p)_i}{dT} \quad (C5)$$

In these equations $(C_p)_i$ is the molar heat capacity of species i , given by equation (81), and C_p is given by equation (16).

Derivatives of the X_s Factors

The formulas for the X_s derivatives depend on the type of chemical reaction being considered. In these equations s is the reaction index.

Type 1 - shuffle reaction. - Differentiating equation (36) and simplifying give the following derivatives:

$$\frac{\partial X_s}{\partial \rho} = 0 \quad (C6)$$

$$\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s \sigma_3 \sigma_4}{K_s} \frac{d \ln K_s}{dT} \quad (C7)$$

The derivative of the rate constant k_s is calculated from equation (33) by logarithmic differentiation

$$\frac{d \ln k_s}{dT} = \frac{n_s}{T} + \frac{E_s}{RT^2} \quad (C8)$$

The equilibrium constant K_s , in concentration units, is given in terms of $(K_p)_s$, the equilibrium constant in terms of partial pressures, by

$$K_s = (K_p)_s (RT)^{-\Delta \nu_s} = e^{-\Delta G_s^0/RT} (RT)^{-\Delta \nu_s} \quad (C9)$$

where $\Delta \nu_s$ is the change in number of moles of species for the reaction and ΔG_s^0 is the standard molar free energy change for the reaction. Logarithmic differentiation of this equation at constant pressure gives

$$\frac{d \ln K_s}{dT} = \frac{\Delta H_s^0}{RT^2} - \frac{\Delta \nu_s}{T} \quad (C10)$$

where ΔH_s^0 is the standard molar enthalpy change for the reaction. Equations (C8) and (C10) hold for all types of reactions being considered.

The remaining X_s derivatives are

$$\frac{\partial X_s}{\partial \sigma_1} = k_s \sigma_2 \quad (C11)$$

$$\frac{\partial X_s}{\partial \sigma_2} = k_s \sigma_1 \quad (C12)$$

$$\frac{\partial X_s}{\partial \sigma_3} = -\frac{k_s \sigma_4}{K_s} \quad (C13)$$

$$\frac{\partial X_s}{\partial \sigma_4} = -\frac{k_s \sigma_3}{K_s} \quad (C14)$$

Type 2a - three-body recombination. - Differentiating equation (37) gives the following derivatives:

$$\frac{\partial X_s}{\partial \rho} = k_s M_s \sigma_1 \sigma_2 \quad (C15)$$

$$\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s M_s \sigma_3}{K_s} \frac{d \ln K_s}{dT} \quad (C16)$$

$$\frac{\partial X_s}{\partial \sigma_1} = k_s \rho M_s \sigma_2 + \frac{X_s m_{1,s}}{M_s} \quad (C17)$$

$$\frac{\partial X_s}{\partial \sigma_2} = k_s \rho M_s \sigma_1 + \frac{X_s m_{2,s}}{M_s} \quad (C18)$$

$$\frac{\partial X_s}{\partial \sigma_3} = -\frac{k_s M_s}{K_s} + \frac{X_s m_{3,s}}{M_s} \quad (C19)$$

Type 2b - two-body dissociation. - Differentiating equation (40) gives the following derivatives:

$$\frac{\partial X_s}{\partial \rho} = - \frac{k_s M_s}{K_s} \sigma_1 \sigma_2 \quad (C20)$$

$$\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s M_s \rho \sigma_1 \sigma_2}{K_s} \frac{d \ln K_s}{dT} \quad (C21)$$

$$\frac{\partial X_s}{\partial \sigma_1} = - \frac{k_s M_s \rho \sigma_2}{K_s} + \frac{X_s m_{1,s}}{M_s} \quad (C22)$$

$$\frac{\partial X_s}{\partial \sigma_2} = - \frac{k_s M_s \rho \sigma_1}{K_s} + \frac{X_s m_{2,s}}{M_s} \quad (C23)$$

$$\frac{\partial X_s}{\partial \sigma_3} = k_s M_s + \frac{X_s m_{3,s}}{M_s} \quad (C24)$$

Type 3a - unimolecular decomposition. - Differentiating equation (41) gives the following derivatives:

$$\frac{\partial X_s}{\partial \rho} = - \frac{k_s \sigma_3}{\rho^2} \quad (C25)$$

$$\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s \sigma_1 \sigma_2}{K_s} \frac{d \ln K_s}{dT} \quad (C26)$$

$$\frac{\partial X_s}{\partial \sigma_1} = - \frac{k_s \sigma_2}{K_s} \quad (C27)$$

$$\frac{\partial X_s}{\partial \sigma_2} = - \frac{k_s \sigma_1}{K_s} \quad (C28)$$

$$\frac{\partial X_s}{\partial \sigma_3} = \frac{k_s}{\rho} \quad (C29)$$

Type 3b - two-body recombination. - Differentiating equation (42) gives the following derivatives:

$$\frac{\partial X_s}{\partial \rho} = \frac{k_s \sigma_3}{\rho^2 K_s} \quad (C30)$$

$$\frac{\partial X_s}{\partial T} = X_s \frac{d \ln k_s}{dT} + \frac{k_s \sigma_3}{\rho K_s} \frac{d \ln K_s}{dT} \quad (C31)$$

$$\frac{\partial X_s}{\partial \sigma_1} = k_s \sigma_2 \quad (C32)$$

$$\frac{\partial X_s}{\partial \sigma_2} = k_s \sigma_1 \quad (C33)$$

$$\frac{\partial X_s}{\partial \sigma_3} = -\frac{k_s}{\rho K_s} \quad (C34)$$

Derivatives of \mathcal{A} and \mathcal{B}

Before differentiating equations (12) and (13) we use equations (8) and (B7) to write \mathcal{A} and \mathcal{B} in the forms

$$\mathcal{A} = M_w \sum_{i=1}^N f_{i+3} - \mathcal{B} \quad (C35)$$

$$\mathcal{B} = M_w \left(\frac{\gamma - 1}{\gamma} \right) \sum_{i=1}^N \left(\frac{h_i}{RT} \right) f_{i+3} \quad (C36)$$

These equations hold for both t and x as the independent variable with the appropriate definitions of the f_{i+3} 's. Now define the quantities

$$S_1 = M_w \sum_{i=1}^N f_{i+3} \quad (C37)$$

$$S_2 = M_w \sum_{i=1}^N \left(\frac{h_i}{RT} \right) f_{i+3} \quad (C38)$$

The equations for \mathcal{A} and \mathcal{B} then become

$$\mathcal{A} = S_1 - \mathcal{B} \quad (C39)$$

$$\mathcal{B} = \left(\frac{\gamma - 1}{\gamma} \right) S_2 \quad (C40)$$

The derivatives of \mathcal{A} and \mathcal{B} are then written in terms of the S_1 and S_2 derivatives as

$$\frac{\partial \mathcal{A}}{\partial V} = \frac{\partial S_1}{\partial V} - \frac{\partial \mathcal{B}}{\partial V} \quad (C41)$$

$$\frac{\partial \mathcal{A}}{\partial \rho} = \frac{\partial S_1}{\partial \rho} - \frac{\partial \mathcal{B}}{\partial \rho} \quad (C42)$$

$$\frac{\partial \mathcal{A}}{\partial T} = \frac{\partial S_1}{\partial T} - \frac{\partial \mathcal{B}}{\partial T} \quad (C43)$$

$$\frac{\partial \mathcal{A}}{\partial \sigma_i} = \frac{\partial S_1}{\partial \sigma_i} - \frac{\partial \mathcal{B}}{\partial \sigma_i} \quad i = 1, 2, \dots, N \quad (C44)$$

$$\frac{\partial \mathcal{B}}{\partial V} = \left(\frac{\gamma - 1}{\gamma} \right) \frac{\partial S_2}{\partial V} \quad (C45)$$

$$\frac{\partial \mathcal{B}}{\partial \rho} = \left(\frac{\gamma - 1}{\gamma} \right) \frac{\partial S_2}{\partial \rho} \quad (\text{C46})$$

$$\frac{\partial \mathcal{B}}{\partial T} = \left(\frac{\gamma - 1}{\gamma} \right) \frac{\partial S_2}{\partial T} + \frac{S_2}{\gamma} \frac{\partial \gamma}{\partial T} \quad (\text{C47})$$

$$\frac{\partial \mathcal{B}}{\partial \sigma_i} = \left(\frac{\gamma - 1}{\gamma} \right) \frac{\partial S_2}{\partial \sigma_i} + \frac{S_2}{\gamma} \frac{\partial \gamma}{\partial \sigma_i} \quad i = 1, 2, \dots, N \quad (\text{C48})$$

Differentiating equations (C37) and (C38) and using the definitions of the $\beta_{i,j}$'s give the following expressions for the S_1 and S_2 derivatives:

$$\frac{\partial S_1}{\partial V} = M_w \sum_{i=1}^N \beta_{i+3,1} \quad (\text{C49})$$

$$\frac{\partial S_1}{\partial \rho} = M_w \sum_{i=1}^N \beta_{i+3,2} \quad (\text{C50})$$

$$\frac{\partial S_1}{\partial T} = M_w \sum_{i=1}^N \beta_{i+3,3} \quad (\text{C51})$$

$$\frac{\partial S_1}{\partial \sigma_j} = M_w \left(\sum_{i=1}^N \beta_{i+3,j+3} - S_1 \right) \quad j = 1, 2, \dots, N \quad (\text{C52})$$

$$\frac{\partial S_2}{\partial V} = M_w \sum_{i=1}^N \left(\frac{h_i}{RT} \right) \beta_{i+3,1} \quad (\text{C53})$$

$$\frac{\partial S_2}{\partial \rho} = M_w \sum_{i=1}^N \left(\frac{h_i}{RT} \right) \beta_{i+3,2} \quad (\text{C54})$$

$$\frac{\partial S_2}{\partial T} = M_w \left[\sum_{i=1}^N \left(\frac{h_i}{RT} \right) \beta_{i+3,3} + \frac{1}{T} \sum_{i=1}^N \frac{(C_p)_i}{R} \right] - \frac{S_2}{T} \quad (C55)$$

$$\frac{\partial S_2}{\partial \sigma_j} = M_w \left[\sum_{i=1}^N \left(\frac{h_i}{RT} \right) \beta_{i+3,j+3} - S_2 \right] \quad j = 1, 2, \dots, N \quad (C56)$$

APPENDIX D

DETAILS OF PROGRAM INPUT AND ERROR MESSAGES

The description of the data cards is divided into three parts. First, the thermodynamic data are described. Next, the complete case data for a single problem are described. We then describe the data cards for any problems following the first. This will show the user how to run several cases at one time without making a complete data deck for each case. Finally an explanation is given for all error messages in the program.

Input Preparation

Thermodynamic data. - The thermodynamic data are not considered part of each case data. The necessary data for all species considered in one computer run are entered before the first case. The first card of the data deck tells where the thermodynamic data will be read from. Columns 1 to 4 of this card must contain either the word CARD or TAPE. If CARD appears, the program reads the data from cards which directly follow the first card. The data are then written out on logical tape unit 4 for use later in the calculation. When TAPE appears on the first data card the thermodynamic data are read from a tape that must be mounted on logical tape unit 4. Each data card corresponds to one logical record on the tape. The format of the thermodynamic data cards is as follows. The first card (or tape record) gives the temperature range limits TLOW, TMID, and THI (in that order) in kelvin units. The card format is 3F10.3. All the thermodynamic data follow this card. They consist of four cards for each species. Card 1 contains the species name, the names of its chemical elements and their stoichiometric coefficients according to the format (2A4, 16X, 4(A2,F3.0)). For example,

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
B2H2C4												B 2. H 2. O 4.																																																																			

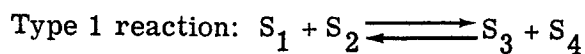
The remaining three cards contain the curve fitted coefficients A_1, A_2, \dots, A_7 of equations (81) to (84) according to the format (5E15.8). Coefficients for the upper temperature range TMID-THI appear first. They are followed by A_1, A_2, \dots, A_7 for the lower range TLOW-TMID. Any number of species data sets may be read in and these can be in any order. The last species data cards must be followed by a card with the word END in columns 1 to 3. The CARD option will generate a permanent thermodynamic data tape,

of course, if a tape is actually mounted on logical tape unit 4.

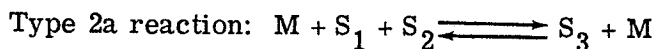
First case data. - The data cards for a single (or first) case are now described in the order they appear in the data deck. All names must be left adjusted in their fields.

(1) Title - The first card of the case data is the title card. The title is read with format (20A4) and printed out at the top of the first page of output.

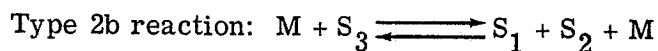
(2) Reactions - Chemical reactions are listed, one per card, in any order. The card contains the participating species names and the rate constant parameters A_j , n_j , and E_j (see eq. (33)) for the forward direction as written. The format of a reaction card is as follows:



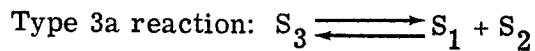
Columns	Contents	Explanation
1 - 8	name of species S_1	-----
10 - 17	name of species S_2	-----
21 - 28	name of species S_3	-----
30 - 37	name of species S_4	-----



1 - 8	name of species S_1	-----
10 - 17	name of species S_2	-----
21 - 28	name of species S_3	-----
30	the letter M	M = third body molecule



1	the letter M	M = third body molecule
10 - 17	name of species S_3	-----
21 - 28	name of species S_1	-----
30 - 37	name of species S_2	-----



1 - 8	blank	-----
10 - 17	name of species S_3	-----
21 - 28	name of species S_1	-----
30 - 37	name of species S_2	-----

Type 3b reaction: $S_1 + S_2 \rightleftharpoons S_3$

Columns	Contents	Explanation
1 - 8	name of species S_1	-----7
10 - 17	name of species S_2	-----
21 - 28	name of species S_3	-----
30 - 37	blank	-----

For all types of reaction the rate constant parameters are listed as follows:

42 - 56	A_j	preexponential factor for k_j in CGS units, format E15.8
59 - 68	n_j	dimensionless temperature exponent, format F10.3
71 - 80	E_j	activation energy in cal/mole, format F10.3

The number of reaction cards may not exceed 30. The end of the reaction list is signalled by a blank card after the last reaction card. The program makes up its own list of reacting species from the species names on the reaction cards. No separate list of reacting species is needed in the data cards.

(3) Inert species - The names of any nonreacting species are listed, four per card, starting in columns 1, 17, 33, and 49. The format is (4(2A4,8X)). The end of the inert species list is signalled by a blank field after the last species name. If there are no inert species, a blank card must be placed here. If there is an exact multiple of four inert species, a blank card must follow the last species card. The total number of inert plus reacting species may not exceed 25.

(4) Version and units - A single card specifies the variable of integration and the assigned variable (pressure or area). It also gives the desired input and output units. Its makeup is as follows:

Columns	Contents	Explanation
1 - 8	TIME	time is the fundamental variable
	DISTANCE	distance is the fundamental variable
	PRESSURE	pressure is assigned
	AREA	area is assigned
11 - 18	blank	velocity is zero, no assigned pressure
21 - 23	CGS or blank	input will be in internal (cgs) units

Columns	Contents	Explanation
	FPS	input will be in FPS units
	SI	input will be in SI units
31 - 33	CGS or blank	output in internal (cgs) units
	FPS	output in FPS units
	SI	output in SI units

(5) Controls - The controls are input through a NAMELIST named PROB. The names of the variables in PROB are given below. If no value for a variable is input (default), then the program uses the standard option for that variable. Standard options are indicated by an underscore.

Name	Value	Explanation
HMIN	-----	minimum step size in cm or sec; values are <u>0.0001 cm</u> or 5.0×10^{-8} sec if defaulted
HMAX	-----	maximum step size in cm or sec; values are <u>0.10 cm</u> or 5.0×10^{-5} sec if defaulted
HINT	-----	initial step size in cm or sec; equal to <u>HMIN</u> , if defaulted
EMAX	-----	maximum allowable relative error per step; equal to <u>0.0001</u> , if defaulted
ALLM1	<u>.TRUE.</u>	all third-body efficiencies are equal to 1; none are input
	.FALSE.	some third-body efficiencies will be read in
ELIM	<u>.TRUE.</u>	automatic elimination from error considerations of species with nonrepresentative errors is desired
	.FALSE.	no automatic eliminations
CONC	<u>.TRUE.</u>	composition is to be output as molar concentrations
	.FALSE.	composition is to be output as mass fractions
EXCHR	.TRUE.	net energy exchange rates are to be output
	<u>.FALSE.</u>	net reaction conversion rates are to be output
ITPSZ	1	an area or pressure table will be input
	2	area or pressure will be specified by polynomial equation.

Name	Value	Explanation
IPRCOD	3	LSUBM and ETA will be input for special area equation, eq. (80)
	4	D, VISC, BETA, and ETA will be input for special area equation, eq. (80)
	<u>5</u>	zero-velocity case - no assigned pressure
	1	distance versus area profile is given
	2	distance versus pressure profile is given
	3	time versus area profile is given
	4	time versus pressure profile is given
XTB	-----	array for time or position half of assigned variable table; must be in user's chosen input units
ATB	-----	array for area or pressure half of assigned variable table; must be in user's chosen input units
NTB	-----	total number of stations in input area or pressure table; must be less than or equal to 40
CX3	-----	coefficient of q^3 in pressure/area equation, (eq. (79))
CX2	-----	coefficient of q^2 in eq. (79)
CX1	-----	coefficient of q in eq. (79)
CX0	-----	constant term in eq. (79)
LSUBM	-----	characteristic shock tube reaction length for special area equation, (eq. (80)) - must be given in cm
ETA	-----	dimensionless exponent in special area equation (eq. (80)) for boundary layer correction
D	-----	hydraulic diameter of shock tube in cm
VISC	-----	viscosity coefficient in g/(cm - sec)
BETA	-----	dimensionless boundary layer parameter used to calculate LSUBM
END	-----	final print station in user's chosen input units; must be a time if time is the fundamental variable and conversely for distance; not needed if array of print stations is input

Name	Value	Explanation
DELP	-----	increment between print stations; same units as END; must not require more than 50 print stations; if defaulted, <u>25 equal increments are taken</u>
PRINT	-----	array of values of the variable of integration at which output is desired; must be in user's chosen input units
APRINT	-----	array of areas or pressures at which output is desired; may only be used if table of assigned pressure or areas is given, and must be in user's chosen input units
NPRNTS	-----	total number of input print stations; must be less than or equal to 50
EVSTEP	.TRUE.	print results after every integration step
	<u>.FALSE.</u>	do not print results after every integration step
DBUGO	.TRUE.	print intermediate output (see p. 38)
	<u>.FALSE.</u>	do not print intermediate output
COMBUS	.TRUE.	perform equilibrium combustion calculations
	<u>.FALSE.</u>	do not perform equilibrium combustion calculations
SHOCK	.TRUE.	perform frozen and equilibrium shock calculations
	<u>.FALSE.</u>	do not perform shock calculations
TCON	.TRUE.	hold temperature constant
	<u>.FALSE.</u>	do not hold temperature constant
RHOCON	.TRUE.	hold volume (density) constant
	<u>.FALSE.</u>	do not hold volume (density) constant

(6) Third-body efficiencies - In order to input third-body efficiencies, the switch ALLM1 must be set to .FALSE. in PROB. If ALLM1 = .TRUE., then there are no input cards from this section. Only those efficiencies which are not equal to 1 actually need to be read in. Three efficiencies can be listed on a single card. The exact card format is

Columns	Contents	Explanation
1 - 37	a dissociation-recombination reaction	these columns must be exactly the same as columns 1 - 37 of the reaction card which contains the same reaction

Name	Value	Explanation
X	-----	axial position
V	-----	velocity
RHO	-----	density
T	-----	temperature
MACH	-----	Mach number
MMHG	.TRUE.	input pressure has units of mm of mercury
	<u>.FALSE.</u>	input pressure is given in the user's chosen input units
MOLEF	<u>.TRUE.</u>	species concentrations will be input as mole fractions
	.FALSE.	species concentrations will be input as mass fractions

(8) Permanently neglected species - The last data for a case are the names of those species which are to be permanently neglected from all error considerations. The neglected species cards have exactly the same format as the inert species cards. They are listed, four per card, starting in card columns 1, 17, 33, and 49. The end of the neglected species list is signalled by a blank field following the last neglected species name. If there are no species to be neglected, then there must be a blank card here. If there is an exact multiple of four neglected species, then the last card containing four names must be followed by a blank card.

(9) Final card - Each case must end with a card containing the word FINIS in card columns 1 to 5.

Multiple cases. - At the end of each case the program tries to read data for another case. Hence, several cases can be computed during one computer run. As mentioned earlier, the program was designed to eliminate the necessity of repeating data which do not change from case to case. This objective was accomplished by adding one switch, named the ACTION switch, to the input list for the second and all following cases of a computer run. By using the ACTION switch the user can tell the program to retain much of the data from the previous case for use by the present case. This means that only those data which change between the present case and the previous case must actually be input. The input cards for each case after the first must correspond to the following specifications. Notice particularly that each case after the first case of a computer run must contain an ACTION card.

(1) Title - The first card of each case data deck must be a title card. The format is the same as before.

(2) ACTION card - The value of the ACTION switch must be punched in columns 1 to 6. The possible values are any one of the words NEW, CHANGE, REPEAT, or ADD.

If the word NEW is input, then the program will completely reinitialize. The remainder of the case data must be exactly like the case data for a first case. The user has told the program not to retain any of the data from the previous case.

The word CHANGE enables the user to change the reaction rate parameters of one or more of the reactions from the previous case. A set of reaction cards, in any order, containing the reaction - written exactly as it was for the previous case - and the new rate parameters must follow the CHANGE card. The end of the change list is signalled by a blank card following the last reaction card. Following the CHANGE list, there must be another ACTION card. This time the options are only ADD or REPEAT.

The REPEAT option tells the program to use the reactions, reaction rates, and inert species which are stored at the time this card is input. If a REPEAT card immediately follows the title card, then the program will use the reactions, reaction rates, and inert species from the previous case. The reactions, unchanged reaction rates, and inert species from the previous case along with the changed reaction rates will be used if the REPEAT card is preceded by a CHANGE list.

The word ADD tells the program to save the reactions, rates, and inert species it has and to prepare to read in one or more additional reactions. A set of reaction cards, again in any order, containing the additional reactions and their reaction rate parameters must follow the ADD card. The end of the add list is signalled by a blank card following the last reaction card. If an ADD card immediately follows the title card, then the program will use the inert species from the previous case along with the reactions from the previous case plus the added reactions. The reactions and inert species from the previous case along with the changed rates and the added reactions will be used if the ADD card is preceded by a CHANGE list.

(3) Version and units - The fundamental variable, input units switch, and output units switch must be reset for each case. The format for this card is the same as before.

(4) Controls - Only those controls which are to be changed from their values in the previous case need to be input. A \$PROB card with no variables listed must still be put in even if no changes are to be made.

(5) Third-body efficiencies - There are no input cards from this section if ALLM1 = .TRUE.. If ALLM1 = .FALSE. then there must be some input cards from this section. The program will use all the third-body efficiencies from the previous case if the only input card from this section is a blank card. The user can change some or all of the efficiencies from the previous case and add new efficiencies by inserting third-body efficiency cards here. Again, the end of the third-body efficiency list is signalled by a blank card.

(6) Initial conditions - All the parameters in NAMELIST START are reinitialized to zero or their standard option before each case. Hence, the input of initial conditions is exactly the same as it was for a first case.

(7) Permanently neglected species - The names of species which are to be permanently neglected from all error considerations are not retained from one case to the next. Hence, a neglected species list must be input for each case. As before, the end of the neglected species list is signalled by a blank field.

(8) Final card - The last card of each case must have the word FINIS in card columns 1 to 5.

Error Messages

Every error message contains two pieces of information: One is the name of the subroutine which generated the message. The second is a statement of the error condition and, whenever possible, a list of the current value of pertinent parameters. Following is a list of the error messages which the program can generate and a brief explanation of each message.

(GCKP)	END OF THIS CASE - READ DATA FOR NEXT CASE	Normal end of case reached
(GCKP)	A FATAL ERROR HAS OCCURRED - CASE TERMINATED	Case ended due to unrecoverable error condition
(KINP)	THE INPUT REACTION LIST DOES NOT CONTAIN THE REACTION $S_1 + S_2 = S_3 + S_4$	Error in entering third-body efficiencies or changing a reaction rate using ACTION switch
(KINP)	THE MASTER SPECIES LIST DOES NOT CONTAIN THE SPECIES ----	The given species is not in the master species list ALSP in the BLOCK DATA
(KINP)	THE INPUT SPECIES LIST DOES NOT CONTAIN THE SPECIES ----	Error in entering third-body efficiencies or permanently neglected species list
(KINP)	INVALID INPUT COMPOSITION SUM = x.xxxx	Input concentrations do not sum to 1.0
(SHOCKS)	EQUILIBRIUM SHOCK CALCULATION FAILED	Iteration of equilibrium shock equations failed to converge

(SHOCKS)	FROZEN SHOCK CALCULATION FAILED	Iteration of frozen shock equations failed to con- verge
(EQLBRM)	DERIVATIVE MATRIX SINGULAR	Singular derivative matrix encountered in equilibrium calculation
(EQLBRM)	SINGULAR MATRIX	Singular matrix encountered in equilibrium calculation
(EQLBRM)	RESTART	Equilibrium calculation re- started
(EQLBRM)	xx ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS	Iteration of equilibrium equations failed to con- verge
(OUTP)	INVALID COMPOSITION	Mass fraction sum not equal to 1.0
(PRED)	WARNING MACH NUMBER = x.xxxx IS APPROACHING 1.0	$0.90 < M < 1.10$; Numerical problems occur if Mach number gets close to 1.0 for assigned area compu- tations
(THRM)	ERROR T = xxxx.xx IS OUT OF RANGE	Temperature (deg K) is above the range of the thermodynamic data
(THRM)	WARNING T = xxxx.xx IS OUT OF RANGE EXTRAPO- LATED VALUES RETURNED	Temperature (deg K) is be- low the range of the ther- modynamic data
(INTE)	RESTART INDEPENDENT VARIA- BLE = xxx.xxx (CGS UNITS) CONTROLLING VARIABLE = ---- H(N-1) H(N) H(N+1) xx.xx xx.xx xx.xx K(N-1) K(N) K(N+1) E(N+1) ---- xx.xx xx.xx xx.xx xx.xx ---- xx.xx xx.xx xx.xx xx.xx	The kinetic calculation is about to be restarted; present location as well as step sizes and results of last 3 steps are given
(INTE)	10 RESTARTS HAVE OCCURRED	Case terminated; too many restarts

(INTE)	COMPOSITION ERROR - NEGATIVE CONCENTRATIONS	The concentration of one or more species is negative
(LESV)	SINGULARITY	Singular coefficient matrix encountered in kinetic calculation
(LESV)	ROW xx OF THE COEFFICIENT MATRIX IS ALL ZEROS xx.xx . . . xx.xx xx.xx . . . xx.xx	Some row of the coefficient matrix is all zeros; the coefficient matrix is given
(CINP)	XI = xx.xx IS OUT OF RANGE X(1) = xx.xx X(N) = xx.xx	Abscissa is out of the range of the assigned variable table; the range of ab- scissas is given

APPENDIX E

TEST CASE DATA AND RESULTS

In this appendix input data and computed results for several kinetics problems are presented. The data are set up as a single computer run to show the use of the multiple-case options CHANGE, ADD, REPEAT, and NEW for the ACTION switch. The data cards used to execute these nine test cases are listed following the case descriptions. Sample listings of results of all cases are then presented. Only selected pages of output are reproduced here, although the input data call for more extensive printout.

Description of Test Cases

Case 1 - This case is the dissociation of Br_2 in a shock tube. It shows the use of the shock option and the Mirels boundary-layer equation (eq. (80)).

Case 2 - This problem is a hydrogen-air ignition and combustion in supersonic flow at constant area. The abbreviated reaction mechanism does not contain the reactions of H_2O_2 with the species H, O, and OH.

Case 3 - This is the same problem as in case 2 and illustrates the use of the CHANGE and ADD options of the ACTION switch. The rate constants for reactions 1 and 3 are changed slightly and three reactions of H_2O_2 are added to the mechanism.

Case 4 - This problem is the same as case 3 with output in FPS units.

Case 5 - This problem is the constant pressure ignition and combustion of methane in a supersonic air stream. It illustrates the use of a unimolecular reaction (reaction 1) and the computation of equilibrium combustion conditions for a constant pressure reaction.

Case 6 - This problem is the same as case 5, with time used as the integration variable. Instead of assigning a constant pressure, we have assigned the area versus distance profile computed in case 5. The computed results do not show perfect agreement with those in case 5 because of curvefitting deviations.

Case 7 - This is another methane-air combustion problem. A pressure profile (in atmospheres) is assigned as a function of distance and output is in SI units. The profile was obtained from the results of a computation which assigned a constant area of 0.10 square meter.

Case 8 - This problem is a constant volume slow reaction of hydrogen and oxygen at a constant temperature of 773 K.

Case 9 - This problem is a high-temperature air ionization reaction in constant area flow. The initial temperature and pressure are generated by a strong shock wave.

Test Case Data Cards

\$DATA
BROMINE DISSOCIATION IN A SHOCK TUBE CASE 1
M +BR2 = BR +BR 6.99E+11 0.50 35500.

XE
DISTANCE AREA
\$PROB ITPSZ=3,ISUBM=32200.,ETA=0.50, SHOCK=.TRUE., END=10.,DELP=0.5,
ALLM1=.FALSE., \$END
M +BR2 = BR +BR BR2 3.80
\$START P=0.1227,MACH=3.2646,T=299.9, BR2=0.01,XE=0.99 \$END

FINIS
H2-AIR SUPERSONIC COMBUSTION (STOICHIOMETRIC) CASE 2
NEW
H2 +OH = H2O +H 2.19E+13 0. 5150.
H +O2 = OH +O 1.25E+14 0. 16300.
O +H2 = OH +H 1.74E+13 0. 9450.
H +O2 = HO2 +M 1.59E+15 0. -1000.
H +H = H2 +M 1.0E+18 -1.0 0.
H2 +HO2 = H2O2 +H 9.60E+12 0. 24000.
M +H2O2 = OH +OH 1.17E+17 0. 45500.
H +HO2 = OH +OH 7.00E+13 0. 0.
H +OH = H2O +M 7.50E+23 -2.60 0.
O +O = O2 +M 1.38E+18 -1. 340.
O +H2O = OH +OH 5.75E+13 0. 18000.
H2 +O2 = OH +OH 1.00E+13 0. 43000.
OH +HO2 = H2O +O2 6.00E+12 0. 0.
O +HO2 = OH +O2 6.00E+12 0. 0.
HO2 +HO2 = H2O2 +O2 1.80E+12 0. 0.

N2
DISTANCE AREA CGS CGS
\$PROB HINT=0.01, ITPSZ=2,CX0=2000., ALLM1=.FALSE., NPRNTS=15,
PRINT=3.048,4.572,6.096,7.620,9.144,12.192,15.24,18.288,21.336,24.384,
27.432,30.48,45.72,60.96,76.20, \$END
H +O2 = HO2 +M H2 5.0 O2 2.0 H2O 32.5
H +O2 = HO2 +M N2 2.0
H +OH = H2O +M H2 4.0 N2 1.6 H2O 20.0
H +OH = H2O +M O2 1.6
H +H = H2 +M O2 2.0 H2 5.0 H2O 15.0
H +H = H2 +M N2 2.0
M +H2O2 = OH +OH O2 0.78 H2O 6.0 H2O2 6.6
M +H2O2 = OH +OH H2 2.3

\$START X=0.,TIME=0.,P=0.9560,T=1559.,MACH=5.03728,
H2=0.2958,O2=0.1480,N2=0.5562 \$END
HO2
FINIS
H2-AIR SUPERSONIC COMBUSTION (COMPLETE MECHANISM - PREFERRED RATES) CASE 3
CHANGE
H2 +OH = H2O +H 2.10E+13 0. 5100.
O +H2 = OH +H 2.96E+13 0. 9800.
ADD
OH +H2O2 = H2O +HO2 1.00E+13 0. 1800.
O +H2O2 = OH +HO2 8.00E+13 0. 1000.
H +H2O2 = H2O +OH 3.18E+14 0. 9000.

DISTANCE AREA
\$PROB \$END
\$START V=455172.99,RHO=1.56283E-04,T=1559.,
H2=0.2958,O2=0.1480,N2=0.5562, \$END
H2C2
FINIS

H2-AIR SUPERSONIC COMBUSTION (OUTPUT IN FPS UNITS) CASE 4

REPEAT
 DISTANCE AREA FPS
 \$PROB \$END

\$START V=455172.99,T=1559.,MDOT=1.42272E+05,
 H2=0.2958,O2=0.1480,N2=0.5562, \$END

HO2 H202

FINIS

METHANE-AIR COMBUSTION AT CONSTANT P (ONE UNIMOLECULAR REACTION) CASE 5

NEW

CH4	= CH3	+H	3.80E+14	0.	103000.
CH4	+O2	= CH3	+HO2	1.00E+13	0.
H	+O2	= HO2	+M	1.59E+15	0.
CO	+O2	= CO2	+O	1.60E+13	0.
CH3	+O2	= CH2O	+OH	7.5E+10	0.
H	+CH4	= CH3	+H2	6.90E+13	0.
O	+CH4	= CH3	+OH	2.00E+13	0.
OH	+CH4	= CH3	+H2O	7.20E+13	0.
H	+O2	= OH	+O	1.25E+14	0.
O	+H2	= OH	+H	2.96E+13	0.
H2	+OH	= H2O	+H	2.10E+13	0.
CO	+OH	= CO2	+H	4.20E+11	0.
CH3	+O	= CH2O	+H	1.90E+13	0.
CH2O	+H	= HCO	+H2	1.00E+13	0.
CH2O	+OH	= HCO	+H2O	7.0E+10	0.70
CH2O	+O	= HCO	+OH	4.00E+11	0.60
HCC	+O	= CO	+OH	1.80E+11	0.50
HCC	+OH	= CO	+H2O	1.10E+11	0.50
HCO	+H	= CO	+H2	1.50E+12	0.50
M	+HCO	= H	+CO	2.00E+13	0.50
HCC	+O2	= CO	+HO2	1.00E+11	0.50
HC2	+HO2	= H2O2	+O2	1.80E+12	0.
H	+HO2	= OH	+OH	7.00E+13	0.
O	+HO2	= OH	+O2	6.00E+12	0.
OH	+HO2	= H2O	+O2	6.00E+12	0.
M	+H2O2	= OH	+OH	1.17E+17	0.
H	+OH	= H2O	+M	7.50E+23	-2.60
M	+O2	= O	+O	2.75E+19	-1.
O	+H2O	= OH	+OH	5.75E+13	0.

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N2

DISTANCE PRESSURE

\$PROB ITPSZ=2, CX0=1.730,HMIN=1.0E-4,HMAX=0.2,HINT=.02,EMAX=.0001,
 PRINT=5.0,10.0,25.0,35.,38.,39.5,40.,40.5,41.,42.,NPRNTS=10,ELIM=.FALSE.,
 COMBUS=.TRUE., ALLM1=.FALSE., \$END

H	+O2	= HO2	+M	CH4	5.0	O2	2.0	N2	2.0
H	+O2	= HO2	+M	H2O	32.5	CO	2.0	CO2	7.5
H	+O2	= HO2	+M			H2	5.0		
M	+H2O2	= OH	+OH	O2	0.78	H2O2	6.6	H2O	6.0
H	+OH	= H2O	+M	N2	1.6	H2O	20.	O2	1.6

\$START AREA=1000.,MACH=2.,T=1645.,
 CH4=0.049768,O2=0.199072,N2=0.75116, \$END

OH HC2 H O
 CO2 H2O2

FINIS

METHANE-AIR COMBUSTION (ASSIGNED AREA - TIME INTEGRATION) CASE 6

REPEAT

TIME AREA

\$PROB ITPSZ=1,IPRCOD=1,HMIN=6.25E-10,HINT=1.25E-7,HMAX=1.25E-6,
 COMBUS=.FALSE., ALLM1=.FALSE., ELIM=.FALSE.,
 XTB=0,5,10,15,20,25,30,35,36,37,38,39,40,40.5,41,42,
 ATB=1000.,1000.45,1002.02,1004.83,1009.24,1016.16,1028.32,1057.02,1068.70,
 1085.55,1112.40,1163.57,1296.55,1371.48,1384.47,1400.45, NTB=16,
 PRINT=6.35273E-5,1.270555E-4,1.90582E-4,2.22346E-4,2.54109E-4,
 2.6615E-04, NPRNTS=6, \$END

\$START P=1.730,V=157412.62,T=1645.,
 CH4=0.049768,O2=0.199072,N2=0.75116, \$END

OH HC2 H O
 CO2 H2O2 HCO

FINIS

METHANE-AIR COMBUSTION (ASSIGNED PRESSURE) CASE 7

RFFEAT
 DISTANCE PRESSURE SI
 \$FROB ITPSZ=1, HMIN=0.0001, HINT=0.02, HMAX=0.20, IPRCOD=2,
 XTB=0., 5., 10., 15., 20., 25., 27.5, 30., 32.5, 35., 35.5, 36., 36.5, 37.0,
 ATB=1.7300, 1.73132, 1.73598, 1.7454, 1.75810, 1.78070, 1.8018, 1.82537,
 1.8718, 1.99243, 2.047, 2.14350, 2.36787, 3.10027, NTR=14,
 PRINT=10., 20., 30., 35., 36.5, NPRPTS=5, ELIM=.FALSE. \$END

\$START AREA=1000., MACH=2., T=1645.,
 CH4=0.049768, O2=0.199072, N2=0.75116, \$END

OH H2 H 0
 CO2 H2O2 CH3

FINIS
 H2-O2 LOW TEMPERATURE REACTION AT CONSTANT VOLUME (ADJUSTED RATES) CASE 8

NEW						
H2	+O2	= H	+HO2	1.00E+14	0.	67000.
H2	+OH	= H2O	+H	2.10E+13	0.	5100.
H	+O2	= OH	+O	1.25E+14	0.	16300.
O	+H2	= OH	+H	2.96E+13	0.	9800.
H	+O2	= HO2	+M	8.50E+14	0.	-1000.
H	+HO2	= OH	+OH	7.00E+13	0.	0.
M	+H2O2	= OH	+OH	1.17E+17	0.	45500.
HO2	+HO2	= H2O2	+O2	1.00E+12	0.	0.
HO2	+H2	= H2O2	+H	8.50E+12	0.	24000.
H	+H2O2	= H2O	+OH	3.18E+14	0.	9000.
OH	+H2O2	= H2O	+HO2	1.00E+13	0.	1800.
O	+H2O	= OH	+OH	5.75E+13	0.	18000.

TIME
 \$FROB HMIN=5.0E-05, HMAX=.1, HINT=.15, EMAX=.0003, ALLM1=.FALSE.,
 RHOCON=.TRUE., TCON=.TRUE., CONC=.FALSE.,
 PRINT=0.75, 1.25, 5., 10., 20., 30., 40., 50., 55., 60., 65., 75., 85., 95.,
 105., 120., NPRPTS=16, \$END

H	+O2	= HO2	+M	H2	5.	O2	2.	H2O	32.5
M	+H2O2	= OH	+OH	H2O	6.	O2	0.78	H2O2	6.6
M	+H2O2	= OH	+OH	H2	2.3				

\$START MMHG=.TRUE., P=500., T=773.15, H2=0.86, O2=0.14, \$END

H OH O HO2

FINIS
 HIGH TEMPERATURE AIR IONIZATION CASE 9

NEW						
N	+O2	= NO	+O	6.43E+09	1.	6250.
O	+N2	= NO	+N	1.36E+14	0.	75400.
N	+O	= NO	+M	6.40E+16	-0.5	0.
O	+O	= O2	+M	1.38E+18	-1.	340.
N	+N	= N2	+M	2.80E+17	-0.75	0.
NO	+O	= NO2	+M	9.40E+14	0.	-1930.
M	+N2O	= N2	+O	5.00E+14	0.	58000.
O	+N2O	= N2	+O2	6.30E+14	0.	26700.
NO+	+E	= N	+O	1.45E+21	-1.5	0.
O+	+E	= O	+M	2.00E+26	-2.5	0.
O2	+E	= O2-	+M	1.52E+21	-1.	1190.
O2	+O-	= O2-	+O	6.00E+12	0.	0.

DISTANCE AREA
 \$FROB HMIN=0.001, HMAX=0.30, ITPSZ=2, CX0=1000., ALLM1=.FALSE.,
 HINT=0.002, DEBUG=.TRUE.,
 PRINT=.02, .04, .06, .08, .10, .30, 1.0, 2.0, 4.0, 10.0, NPRPTS=10 \$END

N	+O	= NO	+M	N2O	2.25
NO	+O	= NO2	+M	N2	1.55
O+	+F	= O	+M	N	0.03 O2 4.5 NO 50.
O+	+E	= O	+M	O	0.03
O2	+E	= O2-	+M	N2	.00002

\$START P=1.6803, V=47002., T=4820., N2=0.7905, O2=0.2095, \$END

NO+ O+ O- O2-

E

FINIS

Selected Test Case Results

** EQUILIBRIUM SHOCK CALCULATION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	0.1227	1.5133	13.1460
VELOCITY (CM/SEC)	57875.78	18108.11	0.3119
DENSITY (GM/CM**3)	6.56092E-04	2.07595E-03	3.1961
TEMPERATURE (DEG K)	299.90	1231.22	4.1054
ENTROPY (CAL/GM/DEG K)	0.3421	0.3576	1.0451
MACH NUMBER	3.2646	0.5171	0.1584
GAFFA	1.6586	1.5731	0.9485
SONIC VELOCITY (CM/SEC)	17728.29	35015.45	1.9751

SPECIES	MOLE FRACTION
BR2	8.12237E-33
BR	3.71905E-33
XE	9.88163E-01

MIXTURE MOLECULAR WEIGHT

131.34058

D(LDG VOLUME)/D(LDG T)
AT CONSTANT P

1.0161

D(LDG VOLUME)/D(LDG P)
AT CONSTANT T

-1.0008

** FROZEN SHOCK CALCULATION **

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	0.1227	1.5017	13.0535
VELOCITY (CM/SEC)	57875.78	18410.72	0.3181
DENSITY (GM/CM**3)	6.56092E-04	2.05248E-03	3.1436
TEMPERATURE (DEG K)	299.90	1245.31	4.1524
ENTROPY (CAL/GM/DEG K)	0.3421	0.3575	1.0449
MACH NUMBER	3.2646	0.5098	0.1562
GAFFA	1.6586	1.6577	0.9994
SONIC VELOCITY (CM/SEC)	17728.29	36115.84	2.0372

SPECIES	MOLE FRACTION
BR2	1.00000E-32
BR	3.
XE	9.90000E-01

MIXTURE MOLECULAR WEIGHT

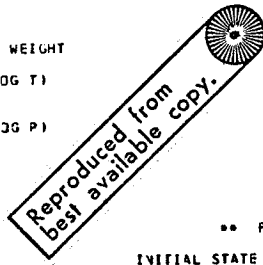
131.58520

D(LDG VOLUME)/D(LDG T)
AT CONSTANT P

1.0000

D(LDG VOLUME)/D(LDG P)
AT CONSTANT T

-1.0000



DISTANCE-AREA VERSION

GENERAL CHEMICAL KINETICS PROGRAM

NASA LEWIS RESEARCH CENTER

BROMINE DISSOCIATION IN A SHOCK TUBE

CASE 1

REACTION
NUMBER

REACTION

REACTION RATE VARIABLES

ACTIVATION

1

M

+ BR2

= BR

+ BR

5.99000E+11

0.5000

EN-RO

35500.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(BR2, 1) = 3.80000

INTEGRATION CONTROLS

MINIMUM STEP SIZE 0.10000E-03 CM

MAXIMUM STEP SIZE 0.10000E+00 CM

INITIAL STEP SIZE 0.10000E-03 CM

MAXIMUM RELATIVE ERROR 0.00010

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION

$$1/AREA = 1 - (X/32200.000)**(0.50000)$$

NO SPECIES WILL BE PERMANENTLY NEGLECTED FROM ALL ERROR CONSIDERATIONS

** INITIAL CONDITIONS **

TIME 0.

SEC

AREA 1.00000E+00 SQ CM

AXIAL POSITION 0.

CM

FLOW PROPERTIES

PRESSURE 1.60167
(ATM)
VELOCITY 18410.72
(CM/SEC)
DENSITY 2.06248E-03
(GM/CM**3)
TEMPERATURE 1243.31
(DEG K)
MASS FLOW RATE 3.79718E+01
(GM/SEC)
ENTROPY 0.3575
(CAL/GM/DEG K)
MACH NUMBER 0.5098
GAMMA 1.6577

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLF FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)	
BR2	1.56741E-07	1.00000E-02	-3.66695E-05	1	8.62032E+00	1.45192E+07	
BR	0.	0.	7.33389E-05				
XE	1.55174E-05	9.90000E-01	0.				
MIXTURE MOLECULAR WEIGHT		131.58920	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)		3.97332E+05	MASS FRACTION SUM 0.99997999	
VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.53658E+03	0.	0.	BR2	-0.93570E-06	0.	0.
RHO	0.17342E+04	0.	0.	BR	0.19314E-05	0.	0.
T	0.50055E+01	0.	0.	XE	0.	0.	0.

TIME 1.03633E-08 SEC

AREA 1.00009E+00 SQ CM

AXIAL POSITION 2.00000E-04 CM

FLOW PROPERTIES

PRESSURE 1.60169
(ATM)
VELOCITY 18410.15
(CM/SEC)
DENSITY 2.06250E-03
(GM/CM**3)
TEMPERATURE 1245.32
(DEG K)
MASS FLOW RATE 3.79740E+01
(GM/SEC)
ENTROPY 0.3575
(CAL/GM/DEG K)
MACH NUMBER 0.5098
GAMMA 1.6577

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 2
AVERAGE STEP SIZE 0.10000E-03
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOL FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
BR2	1.56742E-07	9.99997E-03	-3.65728E-05	1	8.62095E+00	1.45204E+07
BR	7.96730E-13	5.08305E-08	7.33455E-03			
XE	1.55175E-05	9.00000E-01	0.			
MIXTURE MOLECULAR WEIGHT		131.58520	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	3.97352E+05	MASS FRACTION SUM	0.99997999

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.49219E+04	0.	0.	BR2	-3.96581E-05	0.	0.
RHO	0.14500E-03	0.	0.	BR	0.19315E-05	0.	0.
T	0.55698E+02	0.	0.	XE	0.	0.	0.

TIME 2.72460E-05 SEC

AREA 1.00396E+00 SQ CM

AXIAL POSITION 5.00000E-01 CM

FLOW PROPERTIES

PRESSURE 1.60526
(ATM)
VELOCITY 18314.76
(CM/SEC)
DENSITY 2.06614E-03
(GM/CM**3)
TEMPERATURE 1245.82
(DEG K)
MASS FLOW RATE 3.79905E+01
(GM/SEC)
ENTROPY 0.3575
(CAL/GM/DEG K)
MACH NUMBER 0.5070
GAMMA 1.6577

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 14
AVERAGE STEP SIZE 0.35700E-01
CONTROLLING VARIABLE BR
RELATIVE ERROR 0.10910E-05
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOL FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
BR2	1.56016E-07	9.93549E-03	-3.67525E-05	1	8.60932E+00	1.46058E+07
BR	2.00591E-09	1.27742E-04	7.35051E-05			
XE	1.55449E-05	9.99937E-01	0.			
MIXTURE MOLECULAR WEIGHT		131.57660	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	3.96825E+05	MASS FRACTION SUM	0.99997999

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.11920E+03	-0.79370E+01	0.49237E-05	BR2	-0.97124E-06	-0.63706E-07	0.70145E-08
RHO	0.51606E-05	0.34386E-06	0.12564E-06	BR	0.19425E-05	0.12741E-0	0.10910E-05
T	0.15301E+00	0.12302E-01	0.84261E-07	XE	0.	-0.	0.

TIME 3.30791E-04 SEC

AREA 1.01334E+03 SQ CM

AXIAL POSITION 6.00000E+00 CM

FLOW PROPERTIES

PRESSURE 1.61796
(ATM)
VELOCITY 17972.77
(CM/SEC)
DENSITY 2.08495E-03
(GM/CM**3)
TEMPERATURE 1243.53
(DEG K)
MASS FLOW RATE 3.79909E+01
(GM/SEC)
ENTROPY 0.3576
(CAL/GM/DEG K)
MACH NUMBER 0.4977
GAMMA 1.6582

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 6
AVERAGE STEP SIZE 0.94253E-01
CONTROLLING VARIABLE BR
RELATIVE ERROR 0.15103E-06
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLT FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
BR2	1.47046E-07	9.27372E-03	-3.03098E-05	1	6.97257E+00	1.42142E+07
BR	2.28040E-08	1.43817E-03	6.06196E-05			
XE	1.56864E-05	9.89288E-01	0.			

MIXTURE MOLECULAR WEIGHT 131.49058 TOTAL ENERGY EXCHANGE RATE 3.21383E+05 MASS FRACTION SUM 0.99997997
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.44277E+02	-0.29123E+01	0.	BR2	-3.83986E-06	-0.53208E-07	0.117.1E-07
RHO	0.27318E-35	0.17969E-06	0.79355E-09	BR	0.16177E-05	0.10642E-06	0.15103E-06
T	-0.50310E+00	-0.33096E-01	0.77559E-09	XE	0.	-0.	0.

TIME 5.54358E-04 SEC

AREA 1.01794E+03 SQ CM

AXIAL POSITION 1.00000E+01 CM

FLOW PROPERTIES

PRESSURE 1.62368
(ATM)
VELOCITY 17817.78
(CM/SEC)
DENSITY 2.09461E-03
(GM/CM**3)
TEMPERATURE 1241.70
(DEG K)
MASS FLOW RATE 3.79909E+01
(GM/SEC)
ENTROPY 0.3576
(CAL/GM/DEG K)
MACH NUMBER 0.4937
GAMMA 1.6585

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 6
AVERAGE STEP SIZE 0.94264E-01
CONTROLLING VARIABLE BR
RELATIVE ERROR 0.11392E-06
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLT FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
BR2	1.41688E-07	8.89115E-03	-2.34087E-05	1	5.33544E+00	1.39055E+07
BR	3.49906E-08	2.19572E-03	4.68174E-05			
XE	1.57591E-05	9.88913E-01	0.			

MIXTURE MOLECULAR WEIGHT 131.44074 TOTAL ENERGY EXCHANGE RATE 2.45924E+05 MASS FRACTION SUM 0.99997995
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.33939E+02	-0.27321E+01	0.91137E-09	BR2	-0.62722E-06	-0.41322E-07	0.14067E-07
RHO	0.21110E-05	0.13896E-06	0.10486E-08	BR	0.12544E-05	0.82644E-07	0.11392E-06
T	-0.39760E+00	-0.26249E-01	0.40523E-09	XE	0.	-0.	0.

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

H2-AIR SUPERSONIC COMBUSTION

ISTOIC+110METRIC1

CASE 2

REACTION NUMBER	REACTION					REACTION RATE VARIABLES		ACTIVATION ENERGY
	A	N				A	N	
1	H2	+ O2	= H2O	+ H		2.19000E+13	0.	5150.00
2	H	+ O2	= OH	+ O		1.25000E+14	0.	16300.00
3	O	+ H2	= OH	+ H		1.74000E+13	0.	9450.00
4	H	+ O2	= HO2	+ H		1.39000E+15	0.	-1000.00
5	H	+ H	= H2	+ H		1.00000E+18	-1.0000	0.
6	H2	+ H2	= H2O2	+ H		9.60000E+12	0.	24000.00
7	H	+ H2O2	= OH	+ OH		1.17000E+17	0.	45500.00
8	H	+ H2	= OH	+ H		7.30000E+13	0.	0.
9	H	+ H	= H2	+ H		7.50000E+23	-2.6000	0.
10	O	+ O	= O2	+ H		1.38000E+18	-1.0000	340.00
11	O	+ H2O	= OH	+ OH		5.75000E+13	0.	18000.00
12	H2	+ O2	= OH	+ OH		1.00000E+13	0.	43000.00
13	OH	+ H2	= H2O	+ H		6.30000E+12	0.	0.
14	O	+ H2	= OH	+ O2		5.00000E+12	0.	0.
15	HO2	+ H2	= H2O2	+ O2		1.80000E+12	0.	0.

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

MIM2	, 4) =	5.00000	MIM2	, 5) =	5.00000	MIM2	, 7) =	2.30000	MIM2	, 9) =	4.00000
MIM2O	, 4) =	32.50000	MIM2O	, 5) =	15.00000	MIM2O	, 7) =	5.00000	MIM2O	, 9) =	20.00000
MIO2	, 4) =	2.00000	MIO2	, 5) =	2.00000	MIO2	, 7) =	3.78000	MIO2	, 9) =	1.60000
MIM2O2	, 7) =	6.60000	MIM2	, 4) =	2.00000	MIM2	, 5) =	2.00000	MIM2	, 9) =	1.60000

INTEGRATION CONTROLS

MINIMUM STEP SIZE 0.10000E-03 CM
INITIAL STEP SIZE 0.10000E-01 CM

MAXIMUM STEP SIZE 0.10000E+00 CM
MAXIMUM RELATIVE ERROR 0.00010

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

$$\text{AREA (CM**2)} = 1.0. \quad 1X**3 + 1.0. \quad 1X**2 + 1.0. \quad 1X + (2.00000E+03)$$

THE FOLLOWING SPECIES WILL BE NEGLECTED FROM ALL ERROR CONSIDERATIONS

HO2 H2O2

** INITIAL CONDITIONS **

TIME 0. SEC AREA 2.00000E+33 SQ CM AXIAL POSITION 0. CM

FLOW PROPERTIES

PRESSURE 0.95600
(ATM)
VELOCITY 455172.99
(CM/SEC)
DENSITY 1.56283E-04
(GM/CM**3)
TEMPERATURE 1559.00
(DEG K)
MASS FLOW RATE 1.42271E+05
(GM/SEC)
ENTROPY 2.6889
(CAL/GM/DEG K)
MACH NUMBER 5.0373
GAMMA 1.3173

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	2.21055E-06	2.95800E-01	-2.29232E-05	1	0.	4.15419E+12
OH	0.	0.	4.58459E-05	2	0.	6.48455E+11
H2O	0.	0.	0.	3	0.	8.23745E+11
H	0.	0.	5.74772E-10	4	0.	2.19575E+15
O2	1.10602E-06	1.48000E-01	-2.29229E-05	5	-1.17664E-02	6.41437E+14
O	0.	0.	7.75162E-12	6	0.	4.14773E+09
HO2	0.	0.	0.	7	0.	4.89473E+10
H2O2	0.	0.	0.	8	0.	7.00000E+13
H2	4.15645E-06	5.56200E-01	0.	9	0.	3.74681E+15
				10	-1.58687E-04	7.93175E+14
				11	0.	1.72315E+11
				12	9.38528E+02	9.37578E+06
				13	0.	6.00000E+12
				14	0.	6.00000E+12
				15	0.	1.80000E+12

MIXTURE MOLECULAR WEIGHT 20.91269 TOTAL ENERGY EXCHANGE RATE 1.78173E+07 MASS FRACTION SUM 1.00000000
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.17794E+30	0.	0.	4	3.83799E-11	0.	0.
RHO	-0.61096E-10	0.	0.	32	-0.32224E-06	0.	0.
T	-0.19763E-01	0.	0.	0	0.13937E-12	0.	0.
H2	-0.32225E-06	0.	0.	HO2	0.	0.	0.
OH	0.64448E-36	0.	0.	H2O2	0.	0.	0.
H2O	0.	0.	0.	H2	0.	0.	0.

TIME 4.39393E-08 SEC

AREA 2.00000E+03 SQ CM

AXIAL POSITION 2.00000E-02 CM

FLOW PROPERTIES

PRESSURE 0.95600
(ATM)
VELOCITY 455172.99
(CM/SEC)
DENSITY 1.56283E-04
(GM/CM**3)
TEMPERATURE 1559.00
(DEG K)
MASS FLOW RATE 1.42271E+05
(GM/SEC)
ENTROPY 2.5889
(CAL/GM/DEG K)
MACH NUMBER 5.0373
GAMMA 1.3173

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 2
AVERAGE STEP SIZE 0.100J0E-01
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLT FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CJS UNITS)
H2	2.21054E-06	2.45800E-01	-3.82291E-03	1	5.26365E+02	4.15413E+12
OH	1.66596E-12	2.22927E-07	3.08044E-05	2	1.02309E+01	6.46455E+11
H2O	3.52772E-13	4.72055E-08	1.52986E-05	3	3.04087E-01	9.3744E+11
H	3.48412E-13	4.66221E-08	1.50394E-05	4	7.47278E-01	2.19575E+13
O2	1.10602E-06	1.48000E-01	-2.31910E-03	5	-1.17652E-02	6.41637E+14
O	4.07899E-15	5.45822E-10	2.42475E-07	6	1.14834E-04	4.14772E+09
HO2	3.05904E-16	4.19340E-11	1.32492E-08	7	-5.21549E-06	4.49471E+10
H2O2	4.25296E-20	5.69101E-15	2.93216E-12	8	3.03306E-07	7.00000E+13
N2	4.15654E-06	5.96200E-01	0.	9	1.53678E-06	3.74681E+15
				10	-1.58685E-04	7.3177E+14
				11	-5.03564E-04	1.72314E+11
				12	9.38525E+02	9.37575E+06
				13	5.18801E-08	6.10000E+12
				14	-8.90400E-06	6.00000E+12
				15	-1.40853E-11	1.80000E+12

MIXTURE MOLECULAR WEIGHT 20.91269

TOTAL ENERGY EXCHANGE RATE
(CAL-CM**3/GM**2/SEC)

8.44147E+05

MASS FRACTION SUM

0.99997999

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.80274E-01	0.	0.	4	3.21143E-06	0.	0.
RHO	-0.27562E-10	0.	0.	32	-3.32601E-06	0.	0.
T	-0.89073E-02	0.	0.	402	0.34086E-08	0.	0.
H2	-0.53741E-06	0.	0.	4202	0.25554E-09	0.	0.
OH	0.43304E-06	0.	0.		2.41219E-13	0.	0.
H2O	0.21506E-36	0.	0.			0.	0.

TIME 6.67639E-06 SEC

AREA 2.00000E+03 SQ CM

AXIAL POSITION 3.04800E+00 CM

FLOW PROPERTIES

PRESSURE 0.95706
(ATM)
VELOCITY 455157.61
(CM/SEC)
DENSITY 1.56288E-04
(GM/CM**3)
TEMPERATURE 1560.80
(DEG K)
MASS FLOW RATE 1.42271E+05
(GM/SEC)
ENTROPY 2.6913
(CAL/GM/DEG K)
MACH NUMBER 5.0346
GAMMA 1.3172

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 107
AVERAGE STEP SIZE 0.28249E-01
CONTROLLING VARIABLE OH
RELATIVE ERROR 0.14470E-05
PREDICTOR ITERATIONS 3

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLT FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CJS UNITS)
H2	2.19278E-06	2.93436E-01	-1.51295E-02	1	4.34552E+05	4.16215E+12
OH	1.16477E-09	1.55868E-04	1.00807E-03	2	2.59666E+05	6.72401E+11
H2O	1.24390E-08	1.66458E-03	1.06184E-02	3	1.83818E+05	8.6647E+11
H	3.23436E-09	1.23573E-03	7.79068E-03	4	1.96203E+04	2.19493E+15
O2	1.09703E-06	1.46883E-01	-7.08034E-03	5	4.84632E+01	6.40597E+14
O	2.48122E-09	3.32034E-04	2.09182E-03	6	1.42763E+02	4.18494E+09
HO2	3.83507E-10	5.13204E-05	2.18938E-04	7	5.10646E+01	4.97831E+10
H2O2	3.09787E-12	4.14553E-07	2.26052E-05	8	1.01441E+04	7.00000E+13
N2	4.15668E-06	5.56242E-01	0.	9	2.86881E+01	3.73559E+15
				10	1.49224E+00	7.92362E+14
				11	-2.70233E+01	1.73473E+11
				12	9.3878E+02	9.52702E+06
				13	1.09724E+02	6.10000E+12
				14	2.33737E+02	6.00000E+12
				15	1.08369E+01	1.80000E+12

MIXTURE MOLECULAR WEIGHT 20.91425

TOTAL ENERGY EXCHANGE RATE
(CAL-CM**3/GM**2/SEC)

-2.97438E+09

MASS FRACTION SUM

0.99997987

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.31323E+02	-0.34420E+00	0.57912E-10	4	0.10952E-03	0.12195E-05	0.77743E-05
RHO	0.10756E-07	0.11956E-09	0.37935E-10	O2	-0.99533E-04	-0.11083E-06	0.66121E-08
T	0.36492E+01	0.41121E-01	0.14785E-08	2	3.29436E-04	0.32741E-07	0.92056E-06
H2	-0.21257E-03	-0.23680E-05	0.71330E-08	422	0.30778E-05	0.34514E-07	0.11678E-03
OH	0.14171E-04	0.15772E-06	0.14470E-05	4202	0.31779E-07	0.35386E-09	0.25846E-03
H2O	0.14927E-03	0.16519E-05	0.91843E-06	N2	0.	0.	0.

TIME 2.01701E-05 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 9.14400E+00 CM

FLOW PROPERTIES

PRESSURE 1.39443
(ATM)
VELOCITY 448927.62
(CM/SEC)
DENSITY 1.58457E-04
(GM/CM**3)
TEMPERATURE 2343.28
(DEG K)
MASS FLOW RATE 1.42271E+05
(GM/SEC)
ENTROPY 2.7998
(CAL/GM/DEG K)
MACH NUMBER 4.2025
GAMMA 1.2798

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 16
AVERAGE STEP SIZE 0.97496E-01
CONTROLLING VARIABLE JH
RELATIVE ERROR 0.53990E-05
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (C/S UNITS)	
H2	4.87587E-07	6.72339E-02	-1.20323E-03	1	-1.88709E+05	7.24637E+12	
OH	2.51063E-07	3.46193E-02	3.11792E-03	2	1.83474E+04	2.35554E+12	
H2O	1.36430E-06	1.88124E-01	1.24369E-02	3	4.36775E+05	1.70703E+15	
H	5.27396E-07	7.27233E-02	-2.55926E-02	4	1.34559E+05	4.26753E+14	
O2	2.19736E-07	3.02997E-02	-5.35569E-03	5	-1.68178E+03	5.24459E+10	
O	1.87335E-07	2.58319E-02	-4.84476E-03	6	-1.94022E+03	6.67850E+12	
HO2	2.80961E-10	3.87421E-05	-5.96103E-05	7	4.09503E+05	7.00000E+13	
H2O2	3.95829E-11	5.45814E-06	6.62299E-06	8	2.55108E+05	1.49873E+15	
N2	4.21436E-06	5.81123E-01	0.	9	5.54197E+03	5.47650E+14	
				10	-3.76571E+04	1.20457E+12	
				11	-3.58541E+01	9.76180E+08	
				12	1.67112E+04	6.00000E+12	
				13	1.24691E+04	6.00000E+12	
				14	5.33818E+00	1.80000E+12	
				15			
MIXTURE MOLECULAR WEIGHT	21.94979		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	-9.20524E+10	MASS FRACTION SUM	0.99997831	
VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.76043E+03	-0.45553E+02	0.42508E-08	1	-0.35977E-03	-0.21808E-04	0.23055E-06
RHO	0.26841E-06	0.16077E-07	0.42210E-08	2	-3.75289E-04	-0.45500E-05	0.91679E-07
T	0.10118E+03	0.60658E+01	0.89605E-07	3	-0.68105E-04	-0.48912E-05	0.41170E-05
H2	-0.16915E-04	-0.94933E-06	0.27636E-05	402	-0.83798E-07	-0.13355E-07	0.73735E-05
OH	0.43831E-04	0.43244E-05	0.53990E-05	4202	0.33104E-07	-0.43084E-08	0.40276E-04
H2O	0.17483E-03	0.97021E-05	0.45218E-05	N2	0.	-0.	0.

TIME 3.37975E-05 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 1.52400E+01 CM

FLOW PROPERTIES

PRESSURE 1.58450
(ATM)
VELOCITY 446220.20
(CM/SEC)
DENSITY 1.59418E-04
(GM/CM**3)
TEMPERATURE 2712.33
(DEG K)
MASS FLOW RATE 1.42271E+05
(GM/SEC)
ENTROPY 2.8100
(CAL/GM/DEG K)
MACH NUMBER 3.9512
GAMMA 1.2664

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 31
AVERAGE STEP SIZE 0.98579E-01
CONTROLLING VARIABLE 0
RELATIVE ERROR 0.38156E-06
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (C/S UNITS)	
H2	4.61536E-07	6.48287E-02	-2.10895E-03	1	1.10168E+05	8.42318E+12	
OH	2.82740E-07	3.47200E-02	2.82552E-04	2	-3.79320E+04	6.07458E+12	
H2O	1.48200E-06	2.08166E-01	5.71789E-03	3	2.66026E+04	3.01372E+12	
H	3.39764E-07	4.77242E-02	-7.49735E-03	4	1.25122E+05	1.14143E+15	
O2	1.78173E-07	2.50266E-02	-1.85378E-03	5	5.35603E+04	3.86866E+14	
O	1.34988E-07	1.96088E-02	-2.28539E-03	6	-2.33214E+02	1.11800E+11	
HO2	1.37239E-10	1.92770E-05	-4.43152E-06	7	-2.59143E+02	2.52328E+13	
H2O2	1.34439E-11	1.88837E-06	5.35660E-07	8	1.13556E+05	7.00000E+13	
N2	4.23993E-06	5.95553E-01	0.	9	1.23674E+05	8.7911E+14	
				10	2.28574E+03	4.77683E+14	
				11	1.69516E+04	2.33842E+12	
				12	1.09698E+01	3.42941E+09	
				13	8.10259E+03	6.00000E+12	
				14	3.86840E+03	6.00000E+12	
				15	1.04986E+00	1.80000E+12	
MIXTURE MOLECULAR WEIGHT	22.39232		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	-3.35246E+10	MASS FRACTION SUM	0.99997772	
VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.26078E+03	-0.14615E+02	0.26736E-09	1	-0.10543E-03	-0.59330E-05	0.98531E-08
RHO	0.93169E-07	0.52212E-08	0.25590E-09	2	-0.25050E-04	-0.14640E-05	0.13991E-07
T	0.35371E+02	0.20390E+01	0.47343E-08	3	-3.32127E-04	-0.18870E-0	0.38156E-04
H2	-0.29647E-04	-0.16550E-05	0.15951E-07	402	-0.62297E-07	-0.45489E-08	0.14952E-05
OH	0.39720E-05	0.40186E-06	0.36171E-06	4202	0.95388E-08	-0.45243E-07	0.25913E-05
H2O	0.80380E-04	0.44234E-05	0.30578E-07	N2	0.	-0.	0.

TIME 1.79978E-04 SEC

AREA 2.00000E+03 SQ CM

AXIAL POSITION 7.62000E+01 CM

FLOW PROPERTIES

PRESSURE 1.73451
(ATM)
VELOCITY 444082.15
(CM/SEC)
DENSITY 1.60185E-04
(GM/CM**3)
TEMPERATURE 3016.50
(DEG K)
MASS FLOW RATE 1.42270E+05
(GM/SEC)
ENTROPY 2.8125
(CAL/GM/DEG K)
MACH NUMBER 3.7820
GAMMA 1.2566

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 154
AVERAGE STEP SIZE 0.99454E-01
CONTROLLING VARIABLE 0
RELATIVE ERROR 0.38108E-08
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	4.10609E-07	5.85958E-02	-2.18579E-06	1	9.31925E+01	9.27512E+12
OH	2.81530E-07	4.01757E-02	1.66157E-07	2	3.70433E+00	8.24048E+12
H2O	1.60785E-06	2.29448E-01	4.16942E-06	3	2.79116E+01	3.59653E+12
H	2.12931E-07	3.03863E-02	-4.13040E-06	4	5.00161E+01	1.87866E+15
O2	1.43573E-07	2.04886E-02	-1.17052E-06	5	3.59676E+01	3.31510E+14
O	9.06080E-08	1.29302E-02	-1.98892E-05	6	-5.25408E-02	1.75161E+11
H02	5.43539E-11	7.75656E-06	-2.60086E-09	7	-4.43311E-02	5.91081E+13
H2O2	5.81929E-12	8.30440E-07	-2.05164E-10	8	4.36438E+01	7.00000E+13
N2	4.26032E-06	6.07967E-01	0.	9	1.12724E+02	6.73522E+14
				10	1.67811E+00	4.32257E+14
				11	4.83584E+01	2.85458E+12
				12	1.01874E-01	7.66637E+09
				13	4.93436E+00	6.00000E+12
				14	1.59150E+00	6.00000E+12
				15	2.13951E-04	1.80000E+12

MIXTURE MOLECULAR WEIGHT 22.85909 TOTAL ENERGY EXCHANGE RATE -2.23330E+07 MASS FRACTION SUM 0.99999628
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.16405E+00	-0.26850E-02	0.18275E-11	M	-0.58064E-07	-0.90943E-09	0.23010E-09
RHO	0.59176E-10	0.96849E-12	0.18275E-11	O2	-0.15455E-07	-0.29543E-09	0.56095E-09
T	0.23901E-01	0.38975E-03	0.31101E-10	O	-0.27950E-07	-0.32803E-09	0.38108E-08
H2	-0.30727E-07	-0.54917E-09	0.31654E-09	H02	-0.36562E-10	-0.41856E-12	0.32376E-08
OH	0.23358E-08	-0.16866E-09	0.20594E-08	H2O2	-0.28841E-11	-0.48362E-13	0.10198E-07
H2O	0.58613E-07	0.10885E-08	0.24588E-09	N2	0.	-0.	0.

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

H2-AIR SUPERSONIC COMBUSTION (COMPLETE MECHANISM - PREFERRED RATES) CASE 3

REACTION NUMBER	REACTION				REACTION RATE VARIABLES		ACTIVATION ENERGY			
	A	N			A	N				
1	H2	+	J4	=	H2J	+	H	2.10000E+13	0.	5100.00
2	H	+	O2	=	J4	+	O	1.25000E+14	0.	16300.00
3	O	+	H2	=	JH	+	H	2.95000E+13	0.	9800.00
4	H	+	O2	=	H02	+	H	1.59000E+15	0.	-1000.00
5	H	+	H	=	H2	+	H	1.30000E+18	-1.0000	0.
6	H2	+	H32	=	H2O2	+	H	9.60000E+12	0.	24000.00
7	H	+	H2O2	=	JH	+	JH	1.17000E+17	0.	45500.00
8	H	+	H32	=	OH	+	OH	7.00000E+13	0.	0.
9	H	+	J4	=	H2J	+	M	7.50000E+23	-2.6000	0.
10	O	+	O	=	O2	+	M	1.38000E+18	-1.0000	340.00
11	O	+	H2J	=	OH	+	OH	5.75000E+13	0.	18000.00
12	H2	+	J2	=	OH	+	OH	1.00000E+13	0.	43000.00
13	OH	+	H32	=	H2J	+	O2	6.30000E+12	0.	0.
14	O	+	H32	=	JH	+	O2	6.00000E+12	0.	0.
15	H02	+	H32	=	H2O2	+	O2	1.80000E+12	0.	0.
16	OH	+	H2O2	=	H2O	+	H02	1.00000E+13	0.	1800.00
17	O	+	H2O2	=	OH	+	H02	9.00000E+13	0.	1000.00
18	H	+	H2O2	=	H2O	+	OH	3.18000E+14	0.	9000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 4) =	5.00000	M(H2	, 5) =	5.00000	M(H2	, 7) =	2.30000	M(H2	, 9) =	4.00000
M(H2O	, 4) =	32.50000	M(H2J	, 5) =	15.00000	M(H2J	, 7) =	5.00000	M(H2O	, 9) =	20.00000
M(O2	, 4) =	2.00000	M(O2	, 5) =	2.00000	M(O2	, 7) =	0.78000	M(O2	, 9) =	1.60000
M(H2O2	, 7) =	6.60000	M(H2	, 4) =	2.00000	M(H2	, 5) =	2.00000	M(H2	, 9) =	1.60000

INTEGRATION CONTROLS

MINIMUM STEP SIZE 0.10000E-03 CM

MAXIMUM STEP SIZE 0.10000E+00 CM

INITIAL STEP SIZE 0.10000E-01 CM

MAXIMUM RELATIVE ERROR 0.00010

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

$$\text{AREA (CM**2)} = (0. \quad)X**3 + (0. \quad)X**2 + (0. \quad)X + (2.00000E+03)$$

THE FOLLOWING SPECIES WILL BE NEGLECTED FROM ALL ERROR CONSIDERATIONS

H2O2

H02

** INITIAL CONDITIONS **

TIME 0. SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 0. CM

FLOW PROPERTIES

PRESSURE 0.95600
(ATM)
VELOCITY 455172.99
(CM/SEC)
DENSITY 1.56283E-04
(GM/CM**3)
TEMPERATURE 1559.00
(DEG K)
MASS FLOW RATE 1.42272E+05
(GM/SEC)
ENTHALPY 2.6889
(CAL/GM/DEG K)
MACH NUMBER 5.0373
GAMMA 1.3173

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	2.21055E-06	2.95800E-01	-2.29233E-05	1	0.	4.04829E+12
OH	0.	0.	4.58459E-05	2	0.	5.48456E+11
H2O	0.	0.	0.	3	0.	1.25161E+12
H	0.	0.	5.74773E-10	4	0.	2.9575E+15
O2	1.10602E-06	1.48000E-01	-2.29230E-05	5	-1.17664E-02	6.41437E+14
O	0.	0.	7.75164E-12	6	0.	4.14773E+09
H02	0.	0.	0.	7	0.	4.89473E+10
H2O2	0.	0.	0.	8	0.	7.0000E+13
N2	4.15655E-06	5.56200E-01	0.	9	0.	3.74681E+15
				10	-1.58687E-04	7.93176E+14
				11	0.	1.72315E+11
				12	9.38528E+02	9.37578E+06
				13	0.	6.0000E+12
				14	0.	6.0000E+12
				15	0.	1.8000E+12
				16	0.	5.59327E+12
				17	0.	5.79301E+13
				18	0.	1.74082E+13

MIXTURE MOLECULAR WEIGHT 20.91269 TOTAL ENERGY EXCHANGE RATE 1.78173E+07 MASS FRACTION SUM 1.00000000
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.17794E+00	0.	0.	H	0.83799E-11	0.	0.
RHO	-0.61096E-10	0.	0.	O2	-0.32224E-06	0.	0.
T	-0.19763E-01	0.	0.	O	0.13897E-12	0.	0.
H2	-0.32225E-06	0.	0.	H2O	0.	0.	0.
OH	0.64448E-06	0.	0.	H2O2	0.	0.	0.
H2O	0.	0.	0.	N2	0.	0.	0.

TIME 4.39393E-08 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 2.00000E-02 CM

FLOW PROPERTIES

PRESSURE 0.95600
(ATM)
VELOCITY 455172.99
(CM/SEC)
DENSITY 1.56283E-04
(GM/CM**3)
TEMPERATURE 1559.00
(DEG K)
MASS FLOW RATE 1.42272E+05
(GM/SEC)
ENTROPY 2.6889
(CAL/GM/DEG K)
MACH NUMBER 5.0373
GAMMA 1.3173

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 2
AVERAGE STEP SIZE 0.10000E-01
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/S-C)	RATE CONSTANT (CGS UNITS)
H2	2.21055E-06	2.95800E-01	-3.79121E-05	1	6.13243E+02	4.04829E+12
OH	1.67373E-12	2.23967E-07	3.11229E-05	2	1.00060E+01	6.48455E+11
H2O	3.44962E-13	4.61604E-08	1.49781E-05	3	4.45611E-01	1.25161E+12
H	3.40755E-13	4.55974E-08	1.47273E-05	4	7.30855E-01	2.19575E+15
O2	1.10602E-06	1.48000E-01	-2.31851E-05	5	-1.17662E-02	6.41437E+14
O	3.93400E-15	5.26420E-10	2.33527E-07	6	1.12265E-04	4.14772E+09
H2O2	2.99059E-16	4.00180E-11	1.78481E-08	7	-5.29193E-06	4.19471E+10
H2O2	4.16101E-20	5.56797E-15	2.87134E-12	8	2.89887E-07	7.00000E+13
N2	4.15655E-06	5.56200E-01	0.	9	1.51001E-06	3.74681E+15
				10	-1.58685E-04	7.93177E+14
				11	-5.08292E-04	1.72314E+11
				12	9.39524E+02	9.37575E+06
				13	5.12724E-08	6.00000E+12
				14	-8.94554E-06	6.00000E+12
				15	-1.39358E-11	1.80000E+12
				16	1.29632E-11	5.59325E+12
				17	-3.85823E-09	5.79301E+13
				18	1.00917E-11	1.74082E+13

MIXTURE MOLECULAR WEIGHT 20.91269 TOTAL ENERGY EXCHANGE RATE 8.63804E+05 MASS FRACTION SUM 0.99999999
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.82322E-01	0.	0.	H	0.20703E-06	0.	0.
RHO	-0.28265E-10	0.	0.	O2	-0.32593E-06	0.	0.
T	-0.91349E-02	0.	0.	O	0.32828E-08	0.	0.
H2	-0.53295E-06	0.	0.	H2O	0.25090E-09	0.	0.
OH	0.43751E-06	0.	0.	H2O2	0.40364E-13	0.	0.
H2O	0.21056E-06	0.	0.	N2	0.	0.	0.

TIME 6.69641E-06 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 3.04800E+00 CM

FLOW PROPERTIES

PRESSURE 0.95774
(ATM)
VELOCITY 455148.02
(CM/SEC)
DENSITY 1.56291E-04
(GM/CM**3)
TEMPERATURE 1561.92
(DEG K)
MASS FLOW RATE 1.42271E+05
(GM/SEC)
ENTROPY 2.6924
(CAL/GM/DEG K)
MACH NUMBER 5.0329
GAMMA 1.3172

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 110
AVERAGE STEP SIZE 0.27527E-01
CONTROLLING VARIABLE OH
RELATIVE ERROR 0.11939E-06
PREDICTOR ITERATIONS 3

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	2.18292E-06	2.92120E-01	-2.57539E-02	1	7.27382E+05	4.06077E+12
OH	2.00884E-09	2.68824E-04	1.90641E-03	2	4.36048E+05	6.5486E+11
H2O	1.90229E-08	2.54566E-03	1.77848E-02	3	3.25943E+05	1.25904E+12
H	1.49433E-08	2.00000E-03	1.37794E-02	4	3.19688E+04	2.19443E+15
O2	1.09362E-06	1.46348E-01	-1.14402E-02	5	1.27151E+02	6.40237E+14
O	2.90831E-09	3.69259E-04	2.68872E-03	6	1.82151E+02	4.20827E+09
HO2	4.90608E-10	6.56535E-05	2.48277E-04	7	6.36095E+01	5.03107E+10
H2O2	3.46205E-12	4.63295E-07	1.39452E-05	8	2.10120E+04	7.10000E+13
N2	4.15677E-06	5.55262E-01	0.	9	8.03501E+01	3.72861E+15
				10	2.04949E+00	7.91855E+14
				11	-3.37857E+02	1.74198E+11
				12	9.40387E+02	9.62240E+06
				13	2.42077E+02	6.00000E+12
				14	3.50523E+02	6.00000E+12
				15	1.77349E+01	1.80000E+12
				16	1.31867E+00	5.59935E+12
				17	1.62305E+01	5.79651E+13
				18	3.70753E+01	1.75031E+13

MIXTURE MOLECULAR WEIGHT 20.91503 TOTAL ENERGY EXCHANGE RATE -5.34707E+03 MASS FRACTION SUM 0.9999985
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.56251E+02	-0.10022E+01	0.06130E-11	H	0.19371E-03	0.34619E-05	0.89522E-07
RHO	0.19316E-07	0.34414E-09	0.86155E-11	32	-0.15032E-03	-0.28740E-05	0.10741E-08
T	0.66077E+01	0.11773E+00	0.29332E-09	O	0.37797E-04	0.57515E-06	0.10349E-06
H2	-0.36204E-03	-0.64687E-05	0.12220E-08	HO2	0.34902E-05	0.63505E-07	0.95581E-07
OH	0.26800E-04	0.47867E-06	0.11939E-06	H2O2	0.28038E-07	0.50472E-07	0.47332E-07
H2O	0.25001E-03	0.44661E-05	0.99981E-07	N2	0.	-0.	0.

TIME 2.01847E-05 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 9.14400E+00 CM

FLOW PROPERTIES

PRESSURE 1.42431
(ATM)
VELOCITY 448502.09
(CM/SEC)
DENSITY 1.58507E-04
(GM/CM**3)
TEMPERATURE 2400.17
(DEG K)
MASS FLOW RATE 1.42271E+05
(GM/SEC)
ENTRPHY 2.8019
(CAL/GM/DEG K)
MACH NUMBER 4.1598
GAMMA 1.2776

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 16
AVERAGE STEP SIZE 0.95446E-01
CONTROLLING VARIABLE OH
RELATIVE ERROR 0.90493E-05
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLF FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	4.86108E-07	6.72174E-02	-1.80366E-03	1	1.70376E+05	7.20832E+12
OH	2.57962E-07	3.56701E-02	2.73791E-03	2	-1.50387E+05	4.09920E+12
H2O	1.38016E-06	1.90843E-01	1.18571E-02	3	3.61541E+04	3.79266E+12
H	4.96032E-07	6.85897E-02	-2.28401E-02	4	3.77213E+05	1.96089E+15
O2	2.13271E-07	2.94904E-02	-4.89243E-03	5	1.33854E+05	4.18637E+14
O	1.79694E-07	2.48475E-02	-4.79550E-03	6	-9.48364E+02	6.26512E+10
HO2	2.65377E-10	3.65954E-05	-9.96935E-06	7	-3.62213E+04	8.41671E+12
H2O2	2.61287E-11	3.61299E-06	2.64567E-05	8	3.61622E+05	7.10000E+13
N2	4.21836E-06	5.83301E-01	0.	9	2.32610E+05	1.22020E+15
				10	4.95756E+03	5.35399E+14
				11	-2.61045E+04	1.32027E+12
				12	-2.98176E+01	1.21506E+09
				13	1.61218E+04	6.00000E+12
				14	1.12300E+04	6.00000E+12
				15	4.78682E+00	1.80000E+12
				16	1.37441E+03	6.85645E+12
				17	9.05184E+03	6.48685E+13
				18	2.47463E+04	4.81863E+13

MIXTURE MOLECULAR WEIGHT 21.93167 TOTAL ENERGY EXCHANGE RATE -8.48680E+10 MASS FRACTION SUM 0.99999823
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.69424E+03	-0.18836E+02	0.68506E-08	4	-0.32138E-03	-0.87540E-05	0.16148E-07
RHO	0.24551E-06	0.66608E-08	0.68305E-08	32	-0.69776E-04	-0.18714E-05	0.83782E-07
T	0.93029E+02	0.25250E+01	0.14126E-06	O	-0.67413E-04	-0.19337E-05	0.66860E-05
H2	-0.25355E-04	-0.67878E-06	0.26874E-07	HO2	-0.14015E-06	-0.54405E-08	0.20610E-04
OH	0.38489E-04	0.13586E-05	0.90493E-05	H2O2	0.37192E-07	-0.43652E-09	0.89702E-04
H2O	0.16668E-03	0.43796E-05	0.83545E-05	N2	0.	-0.	0.

TIME 3.38210E-05 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 1.52400E+01 CM

FLOW PROPERTIES

PRESSURE 1.59890
(ATM)
VELOCITY 446015.12
(CM/SEC)
DENSITY 1.59491E-04
(GM/CM**3)
TEMPERATURE 2741.00
(DEG K)
MASS FLOW RATE 1.42271E+05
(GM/SEC)
ENTROPY 2.8104
(CAL/GM/DEG K)
MACH NUMBER 3.9340
GAMMA 1.2654

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 32
AVERAGE STEP SIZE 0.97548E-01
CONTROLLING VARIABLE 0
RELATIVE ERROR 0.92294E-06
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)	
H2	6.57874E-07	6.44089E-02	-2.07838E-03	1	9.46637E+04	8.23339E+12	
OH	2.83830E-07	3.9263E-02	2.13917E-04	2	-2.69099E+04	6.26981E+12	
H2O	1.49268E-06	2.09974E-01	5.38597E-03	3	3.53188E+04	4.89670E+12	
H	3.26767E-07	4.59661E-02	-6.82446E-03	4	1.07346E+05	1.41043E+15	
O2	1.74968E-07	2.46120E-02	-1.72021E-03	5	4.81214E+04	3.64830E+14	
O	1.30729E-07	1.83896E-02	-2.15036E-03	6	-1.66417E+02	1.17130E+11	
H02	1.27956E-10	1.79995E-05	-4.47034E-06	7	-1.04953E+04	2.75622E+13	
H2O2	1.17919E-11	1.65877E-06	-7.89514E-08	8	9.88448E+04	7.00000E+13	
N2	4.24188E-06	3.95703E-01	0.	9	1.14145E+05	8.63964E+14	
				10	2.07324E+03	4.72999E+14	
				11	1.32222E+04	2.11089E+12	
				12	1.36369E+01	3.72788E+09	
				13	7.36047E+03	6.00000E+12	
				14	3.39060E+03	6.00000E+12	
				15	8.94259E-01	1.80000E+12	
				16	3.62036E+02	7.18588E+12	
				17	1.54708E+03	6.65820E+13	
				18	8.42682E+03	6.09293E+13	
MIXTURE MOLECULAR WEIGHT	22.43556		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	-3.11599E+13	MASS FRACTION SUM	0.99999766	
VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.24056E+03	-0.55724E+01	0.61330E-09	W	-0.95936E-04	-0.22256E-05	0.49819E-07
RHO	0.86022E-07	0.19926E-08	0.61215E-09	O2	-0.24182E-04	-0.56051E-06	0.19466E-07
T	0.33679E+02	0.78024E+00	0.10550E-07	O	-0.33229E-04	-0.71150E-06	0.92294E-06
H2	-0.29217E-04	-0.67592E-06	0.14283E-07	H02	-0.62842E-07	-0.16160E-08	0.58989E-05
OH	0.30072E-05	0.92711E-07	0.89573E-06	H2O2	-0.11099E-08	-0.12505E-09	0.10158E-04
H2O	0.75714E-04	0.17433E-05	0.83756E-07	N2	0.	0.	0.

TIME 1.71013E-04 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 7.62000E+01 CM

FLOW PROPERTIES

PRESSURE 1.73453
(ATM)
VELOCITY 444081.73
(CM/SEC)
DENSITY 1.60185E-04
(GM/CM**3)
TEMPERATURE 3016.56
(DEG K)
MASS FLOW RATE 1.42270E+05
(GM/SEC)
ENTROPY 2.8125
(CAL/GM/DEG K)
MACH NUMBER 3.7820
GAMMA 1.2566

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 153
AVERAGE STEP SIZE 0.99890E-01
CONTROLLING VARIABLE OH
RELATIVE ERROR 0.29650E-07
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)	
H2	6.10590E-07	5.85943E-02	-2.12821E-05	1	7.90107E+01	8.96859E+12	
OH	2.81528E-07	4.01794E-02	-4.33575E-07	2	4.47305E+00	8.24089E+12	
H2O	1.60788E-06	2.29452E-01	3.63655E-06	3	2.98453E+01	5.77140E+12	
H	2.12911E-07	3.03834E-02	-2.57415E-05	4	3.56666E+01	1.87866E+15	
O2	1.43567E-07	2.04877E-02	-8.79546E-07	5	2.59496E+01	3.31504E+14	
O	9.06003E-08	1.29291E-02	-1.43077E-06	6	-3.41970E-02	1.75174E+11	
H02	5.43442E-11	7.75519E-06	-4.15758E-09	7	-4.55898E+00	5.91164E+13	
H2O2	5.81823E-12	8.30297E-07	-2.39912E-09	8	3.15663E+01	7.00000E+13	
N2	4.26032E-06	6.07969E-01	0.	9	8.13430E+01	6.73490E+14	
				10	1.21036E+00	4.32249E+14	
				11	2.64995E+01	2.85474E+12	
				12	6.92817E-02	7.66738E+09	
				13	3.56952E+00	6.00000E+12	
				14	1.15090E+00	6.00000E+12	
				15	1.59863E-04	1.80000E+12	
				16	1.06989E-01	7.40611E+12	
				17	3.17151E-01	6.77080E+13	
				18	4.19431E+00	7.08560E+13	
MIXTURE MOLECULAR WEIGHT	22.85918		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	-1.68967E+07	MASS FRACTION SUM	0.99999625	
VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.12459E+00	-0.10325E-01	0.28319E-10	W	-0.35137E-07	-0.36315E-08	0.60367E-08
RHO	0.44942E-10	0.37242E-11	0.28319E-10	O2	-0.10929E-08	0.97589E-09	0.23357E-07
T	0.18065E-01	0.15006E-02	0.48202E-09	O	-0.23113E-07	-0.13694E-08	0.64970E-07
H2	-0.29918E-07	-0.19612E-08	0.27038E-09	H02	-0.58446E-10	-0.17104E-11	0.18853E-05
OH	-0.60951E-08	-0.43825E-09	0.29550E-07	H2O2	-0.33726E-10	-0.11321E-12	0.
H2O	0.51122E-07	0.39970E-08	0.21252E-08	N2	0.	0.	0.

(GCKPI) END OF THIS CASE - READ DATA FOR NEXT CASE

H2-AIR SUPERSONIC COMBUSTION

(OUTPUT IN FPS UNITS)

CASE 4

REACTION NUMBER	REACTION	REACTION RATE VARIABLES	ACTIVATION ENERGY
1	H2 + O4 = H2O + 4	2.10000E+13	0.
2	H + O2 = OH + O	1.25000E+14	0.
3	O + H2 = OH + H	2.95000E+13	0.
4	H + O2 = H2O + H	1.59000E+15	0.
5	H + H2 = H2 + H	1.30000E+18	-1.0000
6	H2 + H2 = H2 + H2	9.50000E+12	0.
7	H + H2O2 = OH + H2O	1.17000E+17	0.
8	H + H2 = H2 + H	7.30000E+13	0.
9	H + O4 = H2O + 4	7.50000E+23	-2.6000
10	O + O2 = O3	1.38000E+18	-1.0000
11	O + H2O = OH + H	5.75000E+13	0.
12	H2 + O2 = H2O + H	1.30000E+13	0.
13	OH + H2 = H2O + H	6.00000E+12	0.
14	O + H2 = OH + H	5.30000E+12	0.
15	H2 + O2 = H2O + H	1.80000E+12	0.
16	OH + H2 = H2O + H	1.30000E+13	0.
17	O + H2O2 = OH + H2O	8.00000E+13	0.
18	H + H2O2 = H2O + H	3.18000E+14	0.

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 4) =	5.00000	M(H2	, 5) =	5.00000	M(H2	, 7) =	2.30000	M(H2	, 9) =	4.00000
M(H2O	, 4) =	32.50000	M(H2O	, 5) =	15.00000	M(H2O	, 7) =	5.00000	M(H2O	, 9) =	20.00000
M(O2	, 4) =	2.30000	M(O2	, 5) =	2.00000	M(O2	, 7) =	0.78000	M(O2	, 9) =	1.60000
M(H2O2	, 7) =	6.50000	M(H2O2	, 4) =	2.00000	M(H2O2	, 5) =	2.00000	M(H2O2	, 9) =	1.60000

INTEGRATION CONTROLS

MINIMUM STEP SIZE 0.10000E-03 CM
INITIAL STEP SIZE 0.10000E-01 CM

MAXIMUM STEP SIZE 0.10000E+00 CM
MAXIMUM RELATIVE ERROR 0.00010

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

$$\text{AREA (CM**2)} = (0. \quad)X**3 + (0. \quad)X**2 + (0. \quad)X + (2.00000E+03)$$

THE FOLLOWING SPECIES WILL BE NEGLECTED FROM ALL ERROR CONSIDERATIONS

H2O2 H2O2

** INITIAL CONDITIONS **

TIME	0.	SEC	AREA	2.19278E+00	50 FT	AXIAL POSITION	0.	FT
FLOW PROPERTIES			INTEGRATION INDICATORS					
PRESSURE		2.02309E+03	STEPS FROM LAST PRINT					
(LB/FT**2)			AVERAGE STEP SIZE					
VELOCITY		1.49335E+04	CONTROLLING VARIABLE					
(FT/SEC)			RELATIVE ERROR					
DENSITY		9.75677E-03	PREDICTOR ITERATIONS					
(LB/FT**3)								
TEMPERATURE		2.80620E+03						
(DEG R)								
MASS FLOW RATE		3.13656E+02						
(LR/SEC)								
ENTHALPY		2.68890E+00						
(BTJ/LB/DEG R)								
MACH NUMBER		5.03728E+00						
GAMMA		1.31734E+00						

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-FT**3/LB**2/S C)	RATE CONSTANT (C/S UNITS)
H2	1.38005E-04	2.95800E-01	-1.43111E-03	1	0.	4.04829E+12
OH	0.	0.	2.86218E-03	2	0.	6.44656E+11
H2O	0.	0.	0.	3	0.	1.25161E+12
H	0.	0.	3.58433E-03	4	0.	2.19575E+15
O2	5.90491E-05	1.49000E-01	-1.43109E-03	5	-1.89473E-04	6.41437E+14
O	0.	0.	4.83937E-10	6	0.	4.14773E+09
H2O2	0.	0.	0.	7	0.	4.89673E+10
H2O2	0.	0.	0.	8	0.	7.00000E+13
H2	2.59494E-04	5.36200E-01	0.	9	-2.5413E-06	3.74681E+15
				10	0.	7.93176E+14
				11	0.	1.72315E+11
				12	1.50333E+01	9.77578E+06
				13	0.	6.00000E+12
				14	0.	6.00000E+12
				15	0.	1.80000E+12
				16	0.	5.9327E+12
				17	0.	5.79301E+13
				18	0.	1.74082E+13

MIXTURE MOLECULAR WEIGHT 20.91269 TOTAL ENERGY EXCHANGE RATE 5.13674E+05 MASS FRACTION SUM 1.00000000
(BTU-FT**3/LB**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.17794E+00	0.	0.	4	0.89800E-11	0.	0.
RHO	-0.61096E-10	0.	0.	32	-0.32224E-06	0.	0.
T	-0.19753E-01	0.	0.	3	3.13897E-12	0.	0.
H2	-0.32225E-06	0.	0.	432	0.	0.	0.
OH	0.64449E-06	0.	0.	4202	0.	0.	0.
H2O	0.	0.	0.	N2	0.	0.	0.

TIME 4.39393E-08 SEC AREA 2.15278E+00 SQ FT AXIAL POSITION 6.56168E-04 FT

FLOW PROPERTIES

PRESSURE 2.02309E+03
(LB/FT**2)
VELOCITY 1.49335E+04
(FT/SEC)
DENSITY 9.75677E-03
(LB/FT**3)
TEMPERATURE 2.80620E+03
(DEG R)
MASS FLOW RATE 3.13656E+02
(LB/SEC)
ENTROPY 2.68890E+00
(BTJ/LB/DEG R)
MACH NUMBER 5.03728E+00
GAMMA 1.31734E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 2
AVERAGE STEP SIZE 0.10000E-01
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-FT**3/LB**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	1.38005E-04	2.95800E-01	-2.36687E-03	1	9.82291E+00	4.04829E+12
OH	1.04491E-10	2.23967E-07	1.94301E-03	2	1.60277E-01	6.48455E+11
H2O	2.15362E-11	4.61607E-08	9.35090E-04	3	7.13783E-03	1.25151E+12
H	2.12735E-11	4.55976E-08	9.19433E-04	4	1.17069E-02	2.19575E+15
O2	5.90490E-05	1.48000E-01	-1.44746E-03	5	-1.88471E-04	6.41437E+14
O	2.45602E-13	5.26424E-10	1.45793E-05	6	1.79827E-06	4.14772E+09
H2O2	1.86705E-14	4.00184E-11	1.11427E-05	7	-8.47663E-08	4.39471E+10
H2O2	2.59776E-18	5.56805E-15	1.79260E-10	8	4.64347E-09	7.00000E+13
N2	2.59494E-04	5.56200E-01	0.	9	2.41876E-08	3.74681E+15
				10	-2.54181E-06	7.43177E+14
				11	-8.14182E-06	1.72314E+11
				12	1.50332E+01	9.37575E+06
				13	8.21298E-10	6.00000E+12
				14	-1.43289E-07	6.00000E+12
				15	-2.23242E-13	1.80000E+12
				16	2.07647E-13	5.59326E+12
				17	-6.18016E-11	5.79301E+13
				18	1.61652E-13	1.74082E+13

MIXTURE MOLECULAR WEIGHT 20.91269 TOTAL ENERGY EXCHANGE RATE 2.49034E+05 MASS FRACTION SUM 0.99999999
(BTU-FT**3/LB**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.82322E-01	0.	0.	4	0.20703E-06	0.	0.
RHO	-0.28265E-10	0.	0.	32	-3.32533E-06	0.	0.
T	-0.91349E-02	0.	0.	3	3.32829E-08	0.	0.
H2	-0.53296E-06	0.	0.	H2O2	0.25090E-09	0.	0.
OH	0.43751E-06	0.	0.	4202	0.40365E-13	0.	0.
H2O	0.21056E-06	0.	0.	N2	0.	0.	0.

TIME 6.69641E-06 SEC AREA 2.15278E+00 SQ FT AXIAL POSITION 1.00000E-01 FT

FLOW PROPERTIES

PRESSURE 2.02677E+03
(LB/FT**2)
VELOCITY 1.49327E+04
(FT/SEC)
DENSITY 9.75730E-03
(LB/FT**3)
TEMPERATURE 2.81146E+03
(DEG R)
MASS FLOW RATE 3.13656E+02
(LB/SEC)
ENTROPY 2.69240E+00
(BTJ/LB/DEG R)
MACH NUMBER 5.03290E+00
GAMMA 1.31717E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 110
AVERAGE STEP SIZE 0.27527E-01
CONTROLLING VARIABLE JM
RELATIVE ERROR 0.11939E-06
PREDICTOR ITERATIONS 3

CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-FT**3/LB**2/SEC)	RATE CONSTANT (CGS UNITS)	
H2	1.36290E-04	2.92119E-01	-1.60785E+00	1	1.16514E+04	4.6077E+12	
OH	1.25414E-07	2.68829E-04	1.19020E-01	2	6.98470E+03	6.54870E+11	
H2O	1.18752E-05	2.74570E-03	1.11033E+03	3	5.22103E+03	1.25904E+12	
H	9.33057E-07	2.00003E-03	8.60270E-01	4	5.12084E+02	2.19443E+15	
O2	5.82746E-05	1.46348E-01	-7.14231E-01	5	2.03678E+00	5.40237E+14	
O	1.81600E-07	3.89265E-04	1.67860E-01	6	2.91772E+00	4.20827E+09	
H02	3.06291E-03	6.56543E-05	1.55000E-02	7	1.01890E+00	5.03107E+10	
H2O2	2.15140E-10	4.63301E-07	1.24519E-04	8	3.36530E+02	7.00000E+13	
N2	2.59508E-04	5.55262E-01	0.	9	1.28709E+00	3.72861E+15	
				10	3.28299E-02	7.91855E+14	
				11	-5.41199E+00	1.74198E+11	
				12	1.50631E+01	9.62241E+06	
				13	3.87769E+00	6.00000E+12	
				14	5.61482E+00	6.00000E+12	
				15	2.84084E-01	1.80000E+12	
				16	2.11231E-02	5.59935E+12	
				17	2.59986E-01	5.79651E+13	
				18	5.93888E-01	1.75031E+13	
MIXTURE MOLECULAR WEIGHT		20.91503	TOTAL ENERGY EXCHANGE RATE (BTU-FT**3/LB**2/SEC)		-1.54159E+08	MASS FRACTION SUM	
						0.99999986	

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.56252E+02	-0.10022E+01	0.80139E-11	4	0.19371E-03	0.34520E-05	0.89522E-07
RHO	0.19316E-07	0.34414E-09	0.86172E-11	J2	-0.15033E-03	-0.28740E-05	0.10741E-04
T	0.66078E+01	0.11774E+00	0.29334E-09	J	0.37739E-04	0.57517E-04	0.10349E-06
H2	-0.36205E-03	-0.64688E-05	0.12220E-08	H2O	0.34902E-05	0.63505E-07	0.95532E-07
OH	0.26800E-04	0.47868E-06	0.11939E-06	H2O2	0.29039E-07	0.50472E-09	0.47328E-07
H2O	0.25002E-03	0.44662E-05	0.99983E-07	N2	0.	-0.	0.

TIME 1.71013E-04 SEC AREA 2.15279E+03 SQ FT AXIAL POSITION 2.50000E+00 FT

FLOW PROPERTIES

PRESSURE (LB/FT**2)	3.67063E+03
VELOCITY (FT/SEC)	1.45696E+04
DENSITY (LB/FT**3)	1.00004E-02
TEMPERATURE (DEG R)	5.42980E+03
MASS FLOW RATE (LB/SEC)	3.13653E+02
ENTROPY (BTU/LB/DEG R)	2.81247E+00
MACH NUMBER	3.78200E+00
GAMMA	1.25663E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	153
AVERAGE STEP SIZE	0.99890E-01
CONTROLLING VARIABLE	0
RELATIVE ERROR	0.33940E-07
PREDICTOR ITERATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-FT**3/LB**2/S C)	RATE CONSTANT (CGS UNITS)	
H2	2.56337E-05	5.85943E-02	-1.03549E-04	1	1.01184E+00	8.96859E+12	
OH	1.75798E-05	4.01754E-02	-2.06342E-05	2	1.33329E-01	8.24089E+12	
H2O	1.00340E-04	2.29452E-01	2.32754E-04	3	4.38638E-01	5.77140E+12	
H	1.32920E-05	3.03834E-02	-1.96249E-04	4	5.72672E-01	1.67866E+15	
O2	9.96291E-06	2.04877E-02	-6.12273E-05	5	4.15659E-01	3.11504E+14	
O	5.65619E-06	1.29291E-02	-7.80650E-05	6	-5.48238E-04	1.75174E+11	
H02	3.39272E-09	7.75520E-06	-7.23748E-08	7	-7.43414E-02	5.91164E+13	
H2O2	3.63237E-10	8.30297E-07	-1.29061E-08	8	5.05145E-01	7.00000E+13	
N2	2.65973E-04	6.07969E-01	0.	9	1.30252E+00	6.73490E+14	
				10	1.93759E-02	4.22249E+14	
				11	4.13043E-01	2.85474E+12	
				12	1.13978E-03	7.66739E+09	
				13	5.71222E-02	6.00000E+12	
				14	1.84122E-02	6.00000E+12	
				15	2.55788E-06	1.00000E+12	
				16	1.71343E-03	7.40611E+12	
				17	5.07709E-03	6.77080E+13	
				18	6.71343E-02	7.08550E+13	
MIXTURE MOLECULAR WEIGHT		22.85918	TOTAL ENERGY EXCHANGE RATE (BTU-FT**3/LB**2/SEC)		-4.78930E+05	MASS FRACTION SUM	
						0.99999629	

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.12210E+00	-0.10351E-01	0.22545E-10	4	-0.44193E-07	-0.36126E-08	0.34365E-08
RHO	0.44044E-10	0.37336E-11	0.22545E-10	J2	-0.13797E-07	-0.11081E-08	0.16731E-09
T	0.17782E-01	0.15035E-02	0.38521E-09	J	-0.17574E-07	-0.12961E-06	0.33940E-07
H2	-0.23317E-07	-0.19934E-08	0.14709E-08	H2O	-0.15297E-10	-0.17504E-11	0.76343E-07
OH	-0.40643E-09	-0.56931E-09	0.24413E-07	H2O2	-0.29051E-11	-0.13354E-12	0.15854E-05
H2O	0.45659E-07	0.40834E-08	0.23656E-08	N2	0.	-0.	0.

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

•• EQUILIBRIUM COMBUSTION ••

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	1.7300	1.7300	1.0000
VELOCITY (CM/SEC)	0.	0.	0.
DENSITY (GM/CM**3)	3.61559E-04	2.31911E-04	0.6414
TEMPERATURE (DEG K)	1645.00	2541.98	1.5453
ENTROPY (CAL/GM/DEG K)	2.1308	2.3013	1.0800
MACH NUMBER	0.	0.	0.
GAMMA	1.2777	1.1937	0.9342
SONIC VELOCITY (CM/SEC)	0.	0.	0.
		SPECIES	MOLE FRACTION
		CH4	1.78855E-18
		CH3	2.41035E-17
		H	9.19070E-04
		O2	9.72775E-02
		H2O2	5.47067E-06
		CO	4.90686E-03
		CO2	4.44220E-02
		O	4.17885E-03
		CH2O	8.05191E-12
		OH	1.11270E-02
		H2	1.62431E-03
		H2O	9.10073E-02
		HCO	1.03707E-09
		H2O2	3.02954E-07
		H2	7.44532E-01
MIXTURE MOLECULAR WEIGHT		27.96144	
D(LOG VOLUME)/D(LOG T) AT CONSTANT P		1.0953	
D(LOG VOLUME)/D(LOG P) AT CONSTANT T		-1.0037	

** INITIAL CONDITIONS **

TIME 0. SEC AREA 1.00033E+03 SQ CM AXIAL POSITION 0. CM

FLOW PROPERTIES

PRESSURE 1.73000
(ATM)
VELOCITY 157412.62
(CM/SEC)
DENSITY 3.61559E-04
(GM/CM**3)
TEMPERATURE 1645.00
(DEG K)
MASS FLOW RATE 5.69139E+04
(GM/SEC)
ENTROPY 2.1308
(CAL/GM/DEG K)
MACH NUMBER 2.0000
GAMMA 1.2777

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
CH4	5.37852E-07	4.97680E-02	-5.08397E-06	1	3.83596E+01	7.86161E+00
CH3	0.	0.	5.08397E-06	2	5.31069E-01	4.26588E+04
H	0.	0.	5.01454E-06	3	0.	2.15901E+15
O2	2.55141E-06	1.99072E-01	-6.95166E-08	4	0.	5.1456E+07
HO2	0.	0.	6.94238E-08	5	0.	7.50000E+10
CO	0.	0.	0.	6	0.	1.8697E+12
CO2	0.	0.	0.	7	0.	1.19880E+12
O	0.	0.	1.85618E-10	8	0.	1.18434E+13
CH2O	0.	0.	0.	9	0.	8.93770E+11
OH	0.	0.	0.	10	0.	1.47670E+12
H2	0.	0.	0.	11	0.	4.41213E+12
H2O	0.	0.	0.	12	0.	3.09309E+11
HCO	0.	0.	0.	13	0.	1.90000E+13
H2O2	0.	0.	0.	14	0.	5.42358E+12
N2	9.62725E-06	7.51160E-01	0.	15	0.	9.19511E+12
				16	0.	1.00076E+13
				17	0.	7.30055E+12
				18	0.	4.46145E+12
				19	0.	6.08379E+13
				20	0.	1.28648E+11
				21	0.	7.77419E+11
				22	0.	1.80000E+12
				23	0.	7.00000E+13
				24	0.	6.00000E+12
				25	0.	6.00000E+12
				26	0.	1.05485E+11
				27	0.	3.25859E+15
				28	7.09957E-04	2.83818E+00
				29	0.	2.33475E+11

MIXTURE MOLECULAR WEIGHT 28.21038 TOTAL ENERGY EXCHANGE RATE 4.05133E+05 MASS FRACTION SUM 0.99999999
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.	0.	0.	CO2	0.	0.	0.
RHO	-0.56108E-08	0.	0.	O	0.32514E-11	0.	0.
T	-0.29616E-01	0.	0.	CH2O	0.	0.	0.
CH4	-0.89327E-07	0.	0.	O4	0.	0.	0.
CH3	0.89327E-07	0.	0.	H2	0.	0.	0.
H	0.88108E-07	0.	0.	H2O	0.	0.	0.
O2	-0.12214E-08	0.	0.	HCO	0.	0.	0.
HO2	0.12198E-08	0.	0.	H2O2	0.	0.	0.
CO	0.	0.	0.	N2	0.	0.	0.

TIME 1.59816E-04 SEC

AREA 1.01515E+03 SQ CM

AXIAL POSITION 2.50000E+01 CM

FLOW PROPERTIES

PRESSURE 1.73000
 (ATM)
 VELOCITY 157412.62
 (CM/SEC)
 DENSITY 3.55809E-04
 (GM/CM**3)
 TEMPERATURE 1671.27
 (DEG K)
 MASS FLOW RATE 5.69139E+04
 (GM/SEC)
 ENTRDPY 2.1391
 (CAL/GM/DEG K)
 MACH NUMBER 1.9845
 GAMMA 1.2771

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 76
 AVERAGE STEP SIZE 0.19834E+00
 CONTROLLING VARIABLE HCO
 RELATIVE ERROR 0.33549E-05
 PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MJLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
CH4	5.78219E-07	4.08359E-02	-8.26104E-04	1	5.58913E+01	1.29009E+01
CH3	4.08577E-09	3.23884E-04	8.39991E-05	2	3.35225E-01	5.77537E+04
H	1.62962E-11	1.29182E-06	5.37654E-07	3	-1.62136E+02	2.14865E+15
O2	2.46367E-06	1.95297E-01	-8.03013E-04	4	2.33665E+00	6.45999E+07
HO2	3.30815E-10	2.62240E-05	1.01506E-05	5	5.96346E+03	7.50000E+10
CO	1.72519E-09	1.36757E-04	5.13652E-03	6	1.44898E+02	1.77597E+12
CO2	8.61762E-12	6.83126E-07	5.55506E-07	7	1.65401E+02	1.25302E+12
O	2.89278E-11	2.29313E-06	7.53521E-07	8	6.15949E+03	1.21842E+13
CH2O	4.36535E-08	3.46045E-03	6.96890E-04	9	2.92603E+02	9.73384E+11
OH	1.11328E-10	8.82507E-06	2.01652E-06	10	2.79641E-01	1.54795E+12
H2	8.42517E-10	6.67871E-05	2.19618E-05	11	2.04017E+00	4.52158E+12
H2O	4.81161E-08	3.81421E-03	5.25341E-04	12	4.71455E-01	3.10800E+11
HCO	1.59901E-11	1.26755E-06	5.82771E-07	13	1.77382E+01	1.90000E+13
H2O2	1.14603E-13	9.08471E-09	1.24731E-08	14	3.07701E+01	5.47599E+12
N2	9.47415E-06	7.51024E-01	0.	15	3.58632E+02	9.34248E+12
				16	1.02734E+02	1.29944E+13
				17	2.68861E-02	7.35861E+12
				18	6.32320E-02	4.49693E+12
				19	1.26217E-01	6.13218E+13
				20	2.37059E+02	1.48789E+11
				21	2.50248E+02	8.4217E+11
				22	1.55594E+00	1.50000E+12
				23	2.98082E+00	7.00000E+13
				24	4.52688E-01	6.00000E+12
				25	1.72456E+00	6.00000E+12
				26	1.45742E+00	1.31285E+11
				27	8.23109E-04	3.12708E+15
				28	1.16018E-03	4.74374E+00
				29	2.35792E+00	2.54585E+11

MIXTURE MOLECULAR WEIGHT 28.20529

TOTAL ENERGY EXCHANGE RATE -4.04930E+08
(CAL-CM**3/GM**2/SEC)

MASS FRACTION SUM 0.99999971

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.	0.	0.	CO2	3.53473E-08	0.70033E-09	0.56212E-05
RHO	-0.61662E-06	-0.68605E-07	0.78307E-09	J	0.13454E-07	0.14914E-08	0.59127E-06
T	0.28477E+01	0.31673E+00	0.10421E-08	C42J	0.12407E-04	0.13813E-04	0.30398E-07
CH4	-0.14751E-04	-0.16409E-05	0.45036E-08	O4	0.35004E-07	0.39858E-08	0.33326E-05
CH3	0.12319E-05	0.13655E-06	0.11596E-06	I2	0.39211E-05	0.43371E-07	0.29580E-05
H	0.95996E-08	0.10294E-08	0.30018E-05	H2O	0.16737E-04	0.16389E-03	0.58813E-07
O2	-0.14337E-04	-0.15948E-05	0.10308E-08	HCO	0.10405E-07	0.11271E-08	0.33549E-05
HO2	0.18123E-06	0.20102E-07	0.53903E-07	H2O2	0.22270E-09	0.15353E-10	0.99254E-04
CO	0.10957E-05	0.12107E-06	0.43171E-06	V2	0.	0.	0.

TIME 2.41404E-04 SEC

AREA 1.11240E+03 SQ CM

AXIAL POSITION 3.80000E+01 CM

FLOW PROPERTIES

PRESSURE 1.73000
(ATM)
VELOCITY 157412.62
(CM/SEC)
DENSITY 3.25025E-04
(GM/CM**3)
TEMPERATURE 1618.15
(DEG K)
MASS FLOW RATE 5.69139E+04
(GM/SEC)
ENTROPY 2.1861
(CAL/GM/DEG K)
MACH NUMBER 1.8973
GAMMA 1.2765

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 27
AVERAGE STEP SIZE 0.11158E+00
CONTROLLING VARIABLE HCO
RELATIVE ERROR 0.38975E-04
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOL FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CSS UNITS)
CH4	2.76755E-07	2.58720E-02	-1.26977E-02	1	-4.13987E+03	1.58028E+02
CH3	5.31935E-08	4.58797E-03	3.45175E-03	2	-1.12356E+02	2.67378E+05
H	1.63519E-09	1.41031E-04	2.40719E-04	3	-1.40366E+04	2.09701E+15
O2	1.99855E-06	1.72378E-01	-1.35405E-02	4	3.18726E+02	1.8587E+08
H2O2	5.82420E-09	5.08570E-04	2.17622E-04	5	7.54810E+04	7.30000E+10
CO	3.92853E-08	7.70063E-03	8.27224E-03	6	9.80359E+03	2.53292E+12
CO2	9.21151E-10	7.44469E-05	1.22939E-04	7	5.08935E+03	1.76729E+12
O	1.25851E-09	1.08543E-04	1.50398E-04	8	1.09555E+05	1.40545E+13
CH2O	1.51727E-07	1.30861E-02	6.96665E-04	9	4.21275E+04	1.37271E+12
OH	3.14395E-09	2.71158E-04	4.11843E-04	10	5.72273E+02	1.96467E+12
H2	2.76627E-08	2.48584E-03	2.29540E-03	11	2.46386E+03	5.11890E+12
H2O	3.27487E-07	2.82449E-02	1.67108E-02	12	8.45008E+02	3.18453E+11
HCO	1.48625E-09	1.28195E-04	1.54067E-04	13	1.20407E+04	1.90000E+13
H2O2	1.62901E-11	1.40498E-06	1.66410E-06	14	1.34988E+04	5.74899E+12
N2	3.65447E-06	7.46426E-01	0.	15	4.58460E+04	1.01539E+13
				16	2.15822E+04	1.19404E+13
				17	1.35894E+02	7.67516E+12
				18	2.07463E+02	4.69038E+12
				19	1.47140E+03	6.39597E+13
				20	5.07584E+04	3.11172E+11
				21	2.68955E+04	9.76558E+11
				22	7.93468E+02	1.80000E+12
				23	7.39404E+03	7.00000E+13
				24	4.87690E+02	6.00000E+12
				25	1.21774E+03	6.00000E+12
				26	7.77716E+02	3.47089E+11
				27	2.94476E+00	2.51202E+15
				28	-8.54764E-02	8.15539E+01
				29	1.10858E+03	3.74448E+11

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MIXTURE MOLECULAR WEIGHT	28.03260	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	-7.94840E+09	MASS FRACTION SUM	0.99999977		
VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.	-0.	0.	CO2	0.24029E-05	0.20514E-06	0.77609E-04
RHO	-0.10217E-04	-0.89754E-06	0.75298E-06	O	0.29513E-05	0.25078E-06	0.88250E-04
T	0.50690E+02	0.44376E+01	0.80956E-06	CH2O	0.13617E-04	0.14195E-05	0.94955E-05
CH4	-0.24818E-04	-0.21901E-04	0.41274E-05	OH	0.80496E-05	0.65920E-06	0.11139E-03
CH3	0.67466E-04	0.59716E-05	0.32071E-05	H2	0.44884E-04	0.39209E-05	0.15830E-04
H	0.47049E-05	0.36519E-06	0.11674E-03	H2O	0.32552E-03	0.28547E-04	0.86454E-05
O2	-0.26455E-03	-0.23258E-04	0.98457E-05	HCO	0.30113E-05	0.26862E-06	0.38975E-04
H2O2	0.42536E-05	0.42173E-06	0.29646E-04	H2O2	0.32525E-07	0.58875E-09	0.13681E-03
CO	0.16168E-03	0.14036E-04	0.25572E-04	N2	0.	-0.	0.

TIME 2.50933E-04 SEC

AREA 1.21259E+03 SQ CM

AXIAL POSITION 3.95000E+01 CM

FLOW PROPERTIES

PRESSURE 1.73000
(ATM)
VELOCITY 157412.62
(CM/SEC)
DENSITY 2.98146E-04
(GM/CM**3)
TEMPERATURE 1959.63
(DEG K)
MASS FLOW RATE 5.69139E+04
(GM/SEC)
ENTROPY 2.2310
(CAL/GM/DEG K)
MACH NUMBER 1.8158
GAMMA 1.2787

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 26
AVERAGE STEP SIZE 0.61148E-01
CONTROLLING VARIABLE HCO
RELATIVE ERROR 0.17799E-04
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
CH4	8.96005E-08	8.33100E-03	-2.28911E-02	1	-4.42863E+04	1.23761E+03
CH3	8.61361E-08	8.00887E-03	9.91434E-04	2	-2.09712E+02	9.41563E+05
H	9.74121E-09	8.12752E-04	2.36965E-03	3	-3.52650E+04	2.05553E+15
O2	1.62461E-06	1.51055E-01	-3.95226E-02	4	1.88719E+03	4.28101E+08
H2O	5.95192E-09	5.53406E-04	-6.47244E-04	5	1.18070E+05	7.50000E+10
CO	2.41245E-07	2.24308E-02	3.31094E-02	6	2.15503E+04	3.33304E+12
CO2	5.45722E-09	5.07408E-04	1.63593E-03	7	1.21874E+04	1.88360E+12
O	5.96839E-09	6.47917E-04	2.35485E-03	8	2.68278E+05	1.58244E+13
CH2O	9.95371E-08	9.25490E-03	-1.31231E-02	9	2.90260E+05	1.90122E+12
OH	1.88113E-08	1.74906E-03	5.83533E-03	10	7.91588E+03	2.38965E+12
H2	5.00369E-08	5.58219E-03	4.88511E-03	11	4.33624E+04	5.66808E+12
H2O	5.65220E-07	5.25537E-02	4.86171E-02	12	1.65166E+04	3.24880E+11
HCO	4.00419E-09	3.72307E-04	2.77462E-04	13	1.28296E+05	1.90000E+13
H2O2	5.62114E-12	6.15629E-07	-1.60565E-06	14	5.85382E+04	5.98339E+12
N2	7.93875E-06	7.38140E-01	0.	15	2.29910E+05	1.09167E+13
				16	1.05550E+05	1.35288E+13
				17	2.50121E+03	7.96818E+12
				18	4.12626E+03	4.86944E+12
				19	2.61461E+04	6.64015E+13
				20	2.77156E+05	5.72094E+11
				21	8.09468E+04	1.10623E+12
				22	7.17328E+02	1.80000E+12
				23	4.09693E+04	7.00000E+13
				24	2.79791E+03	6.00000E+12
				25	7.55152E+03	6.00000E+12
				26	7.35391E+02	9.85698E+11
				27	1.03840E+02	2.06733E+15
				28	-3.11514E+00	8.10959E+02
				29	6.40109E+03	5.65192E+11

MIXTURE MOLECULAR WEIGHT 27.72139

TOTAL ENERGY EXCHANGE RATE -3.05072E+10
(CAL-CM**3/GM**2/SEC)

MASS FRACTION SUM 1.00000010

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.	-0.	0.	CO2	3.34958E-04	0.91590E-06	0.64862E-05
RHO	-0.31309E-04	-0.84125E-06	0.66504E-08	O	3.53176E-04	0.12524E-05	0.22061E-04
T	0.17813E+03	3.47614E+01	0.69262E-07	CH2O	-0.27962E-03	-0.74928E-05	0.10099E-05
CH4	-0.48775E-03	-0.13289E-04	0.33298E-05	O	0.12434E-03	0.33226E-05	0.86878E-05
CH3	0.21125E-04	0.76102E-06	0.45417E-05	H2	3.10403E-03	0.28474E-05	0.14193E-05
H	0.50491E-04	0.13078E-05	0.86646E-05	H2O	3.10359E-02	0.27846E-04	0.17071E-06
O2	-0.84213E-03	-0.22578E-04	0.91784E-07	HCO	0.59120E-05	0.19574E-06	0.17799E-04
H2O	-0.13791E-04	-0.35341E-06	0.42568E-05	H2O2	-0.34212E-07	-0.82516E-09	0.19100E-05
CO	0.70548E-03	0.18909E-04	0.11689E-06	N2	3.	-0.	0.

TIME 2.54109E-04 SEC AREA 1.29559E+03 SQ CM AXIAL POSITION 4.00000E+01 CM

FLOW PROPERTIES

PRESSURE 1.73000
(ATM)
VELOCITY 157412.62
(CM/SEC)
DENSITY 2.78854E-04
(GM/CM**3)
TEMPERATURE 2070.66
(DEG K)
MASS FLOW RATE 5.69139E+04
(GM/SEC)
ENTROPY 2.2632
(CAL/GM/DEG K)
MACH NUMBER 1.7551
GAMMA 1.2804

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 14
AVERAGE STEP SIZE 0.37656E-01
CONTROLLING VARIABLE HCO
RELATIVE ERROR 0.65701E-04
PREDICTOR ITERATIONS C

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOL. FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (GKS UNITS)
CH4	2.22181E-08	2.18976E-03	-1.37339E-02	1	-7.92512E+04	5.49523E+03
CH3	5.82792E-08	5.74383E-03	-1.81727E-02	2	-8.48341E+01	2.14332E+06
H	2.04000E-08	2.01056E-03	5.59890E-03	3	-2.50956E+04	2.02599E+15
O2	1.36036E-06	1.34073E-01	-6.44029E-02	4	4.70716E+03	7.74906E+08
H2O	2.39944E-09	2.35465E-04	-9.47909E-04	5	7.64672E+04	7.50000E+10
CO	1.60579E-08	3.42779E-02	4.24721E-02	6	1.53421E+04	3.35374E+12
CO2	2.34900E-08	1.58262E-03	6.61424E-03	7	1.18183E+04	2.15187E+12
O	4.36895E-08	4.30591E-03	1.23063E-02	8	2.29440E+05	1.72350E+13
CH2O	5.50120E-08	5.42182E-03	-1.64723E-02	9	7.05919E+05	2.40705E+12
OH	6.42010E-08	6.32747E-03	1.62080E-02	10	2.43770E+04	2.75380E+12
H2	7.03032E-07	6.92888E-02	-1.45571E-03	11	1.50246E+05	6.10227E+12
H2O	3.90309E-09	3.84677E-04	6.15943E-02	12	8.03532E+04	3.29616E+11
HCO	7.10135E-12	6.99889E-07	-6.56871E-04	13	3.34501E+05	1.90000E+13
H2O2	7.42506E-06	7.31792E-01	1.10277E-05	14	7.05516E+04	5.15912E+12
N2			0.	15	3.56430E+05	1.15349E+13
				16	1.95850E+05	1.44428E+13
				17	9.67151E+03	8.20258E+12
				18	1.38417E+04	5.1275E+12
				19	6.99957E+04	6.83557E+13
				20	4.33686E+05	8.90897E+11
				21	8.40658E+04	1.23135E+12
				22	1.94163E+02	1.0000E+12
				23	5.31728E+04	7.00000E+13
				24	5.23971E+03	6.00000E+12
				25	1.22748E+04	6.00000E+12
				26	5.23441E+01	1.90428E+12
				27	7.36153E+02	1.77791E+15
				28	-3.74661E+01	4.26470E+03
				29	-2.91457E+04	7.33389E+11

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MIXTURE MOLECULAR WEIGHT 27.48301 TOTAL ENERGY EXCHANGE RATE -5.19924E+10 MASS FRACTION SUM 1.00000054
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.	-0.	0.	CO2	0.15068E-03	0.32848E-05	0.94848E-05
RHO	-0.43372E-04	-0.97549E-06	0.62199E-05	O	0.28035E-03	0.56441E-05	0.67115E-04
T	0.28268E+03	0.63143E+01	0.40958E-06	CH2O	-0.37523E-03	-0.85212E-05	0.15995E-04
CH4	-0.31402E-03	-0.73159E-05	0.30523E-04	O4	0.41481E-03	0.98868E-05	0.33422E-04
CH3	-0.41400E-03	-0.90190E-05	0.56303E-04	H2	-0.33185E-04	-0.81347E-05	0.25278E-05
H	0.12483E-03	0.28987E-05	0.11295E-04	CO	0.14032E-02	0.31271E-05	0.11412E-05
O2	-0.14672E-02	-0.32724E-04	0.37286E-05	HCO	-0.14955E-04	-0.24833E-06	0.65731E-04
H2O	-0.21495E-04	-0.48910E-06	0.10321E-04	H2O2	0.25123E-06	0.15323E-04	0.49192E-03
CO	0.96758E-03	0.21621E-04	0.37598E-05	N2	0.	-0.	0.

** INITIAL CONDITIONS **

TIME 0. SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 0. CM

FLOW PROPERTIES

PRESSURE 1.73000
(ATM)
VELOCITY 157412.62
(CM/SEC)
DENSITY 3.61559E-04
(GM/CM**3)
TEMPERATURE 1645.00
(DEG K)
MASS FLOW RATE 5.69139E+04
(GM/SEC)
ENTROPY 2.1308
(CAL/GM/DEG K)
MACH NUMBER 2.0000
GAMMA 1.2777

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.
CONTROLLING VARIABLE

RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
CH4	5.37852E-07	4.97680E-02	-5.08397E-06	1	3.83596E+01	7.86161E+00
CH3	0.	0.	5.08397E-06	2	5.31069E-01	4.26588E+04
H	0.	0.	5.01454E-06	3	0.	2.15931E+15
O2	2.55141E-06	1.99072E-01	-6.95166E-08	4	0.	5.71456E+07
HO2	0.	0.	6.94238E-08	5	0.	7.50000E+10
CO	0.	0.	0.	6	0.	1.86697E+12
CO2	0.	0.	0.	7	0.	1.19880E+12
O	0.	0.	1.85618E-10	8	0.	1.18434E+13
CH2O	0.	0.	0.	9	0.	8.53770E+11
OH	0.	0.	0.	10	0.	1.47670E+12
H2	0.	0.	0.	11	0.	4.41213E+12
H2O	0.	0.	0.	12	0.	3.09309E+11
HCO	0.	0.	0.	13	0.	1.90000E+13
H2O2	0.	0.	0.	14	0.	5.42358E+12
N2	9.62725E-06	7.51160E-01	0.	15	0.	9.19511E+12
				16	0.	1.00076E+13
				17	0.	7.30055E+12
				18	0.	4.46145E+12
				19	0.	6.08379E+13
				20	0.	1.28648E+11
				21	0.	7.77419E+11
				22	0.	1.80000E+12
				23	0.	7.00000E+13
				24	0.	6.00000E+12
				25	0.	6.00000E+12
				26	0.	1.05485E+11
				27	0.	3.25859E+15
				28	7.09957E-04	2.33818E+00
				29	0.	2.33676E+11

MIXTURE MOLECULAR WEIGHT 28.21038 TOTAL ENERGY EXCHANGE RATE 4.05133E+06 MASS FRACTION SUM 0.99999999
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.13341E+07	0.	0.	CO2	0.	0.	0.
RHO	-0.11374E-01	0.	0.	O	0.51338E-06	0.	0.
T	-0.20149E+05	0.	0.	CH2O	0.	0.	0.
CH4	-0.14061E-01	0.	0.	OH	0.	0.	0.
CH3	0.14061E-01	0.	0.	H2	0.	0.	0.
H	0.13869E-01	0.	0.	H2O	0.	0.	0.
O2	-0.19227E-03	0.	0.	HCO	0.	0.	0.
HO2	0.19201E-03	0.	0.	H2O2	0.	0.	0.
CO	0.	0.	0.	N2	0.	0.	0.

TIME 1.0582E-04 SEC

AREA 1.02832E+03 SQ CM

AXIAL POSITION 3.00003E+01 CM

FLOW PROPERTIES

PRESSURE 1.72995
(ATM)
VELOCITY 157413.11
(CM/SEC)
DENSITY 3.51599E-04
(GM/CM**3)
TEMPERATURE 1690.78
(DEG K)
MASS FLOW RATE 5.69138E+04
(GM/SEC)
ENTHALPY 2.1450
(CAL/GM/DEG K)
MACH NUMBER 1.9730
GAMMA 1.2768

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 51
AVERAGE STEP SIZE 0.12433E-05
CONTROLLING VARIABLE CO
RELATIVE ERROR 0.15437E-04
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
CH4	5.35541E-07	4.29493E-02	-1.57047E-03	1	5.16923E+01	1.34509E+01
CH3	7.63777E-09	6.12534E-04	1.85196E-04	2	-9.49360E-01	7.18833E+04
H	5.15450E-11	4.13380E-06	2.37953E-06	3	-5.56575E+02	2.14120E+15
O2	2.39960E-06	1.92443E-01	-1.53312E-03	4	8.6311E+00	8.32537E+07
H2O	9.19162E-10	7.7149E-05	3.19255E-05	5	1.1111E+04	7.50000E+10
CO	5.54094E-09	4.44372E-04	2.21041E-04	6	4.43636E+02	2.05865E+12
CO2	3.24448E-11	2.60602E-06	1.44899E-06	7	4.12629E+02	1.24365E+13
O	7.37294E-11	5.91295E-06	2.52870E-06	8	1.17818E+04	9.77179E+11
CH2O	7.14738E-09	5.73205E-03	1.16021E-03	9	9.75512E+00	1.50157E+12
OH	2.21062E-10	1.77287E-05	6.08237E-06	10	1.93356E+00	4.60250E+12
H2	2.15126E-09	1.72327E-04	7.45023E-05	11	9.78125E+00	3.11881E+11
H2O	9.37742E-08	6.71852E-03	1.60685E-03	12	3.08953E+00	1.90000E+13
HCO	5.50241E-11	4.41282E-06	2.57582E-06	13	8.55496E+01	5.51417E+12
H2O2	7.45522E-13	5.97893E-08	1.06744E-07	14	1.54325E+02	9.45146E+12
N2	9.36207E-06	7.50819E-01	0.	15	1.20717E+03	1.05165E+13
				16	4.48294E+02	4.52310E+12
				17	2.42892E-01	7.40143E+12
				18	4.45046E-01	4.52310E+12
				19	1.41507E+00	6.16786E+13
				20	9.17348E+02	1.65288E+13
				21	8.40307E+02	8.24214E+11
				22	1.23011E+01	1.80000E+12
				23	2.68275E+01	7.00000E+13
				24	3.28712E+00	6.00000E+12
				25	9.81516E+00	6.00000E+12
				26	1.14376E+01	1.53766E+11
				27	5.62737E-03	3.03414E+15
				28	1.43857E-03	7.38072E+00
				29	1.17547E+01	2.71013E+11

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MIXTURE MOLECULAR WEIGHT 28.19756

TOTAL ENERGY EXCHANGE RATE -7.75862E+08
(CAL-CM**3/GM**2/SEC)

MASS FRACTION SUM 0.99999967

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.19933E+07	-0.21421E+01	0.21930E-07	C2	0.41211E-02	0.46564E-08	0.19993E-04
RHO	-0.16429E+00	-0.18964E-06	0.14624E-07	3	0.71920E-02	0.82519E-08	0.15535E-04
T	0.87051E+06	0.99684E+00	0.93622E-07	C2O	0.32998E+01	0.37958E-05	0.12590E-05
CH4	-0.44666E+01	-0.51203E-04	0.43379E-06	H	0.17299E-01	0.19432E-07	0.11456E-04
CH3	0.52673E+00	0.69822E-04	0.70957E-05	H2	0.21190E+00	0.24019E-07	0.13051E-04
H	0.67677E-02	0.71047E-08	0.33371E-04	H2O	0.45701E+01	0.23555E-05	0.30807E-05
O2	-0.43604E+01	-0.49985E-05	0.95315E-07	CO	0.73250E-02	0.78790E-08	0.30349E-04
H2O	0.90801E-01	0.10410E-06	0.90235E-05	CO2	0.30359E-03	0.15156E-07	0.21175E-03
CO	0.62867E+00	0.71215E-06	0.15487E-04	N2	0.	-0.	0.

TIME 2.22346E-04 SEC

AREA 1.05702E+03 SQ CM

AXIAL POSITION 3.49997E+01 CM

FLOW PROPERTIES

PRESSURE 1.73004
(ATM)
VELOCITY 157411.87
(CM/SEC)
DENSITY 3.42061E-04
(GM/CM**3)
TEMPERATURE 1735.81
(DEG K)
MASS FLOW RATE 5.69145E+04
(GM/SEC)
ENTHALPY 2.1590
(CAL/GM/DEG K)
MACH NUMBER 1.9454
GAMMA 1.2763

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 27
AVERAGE STEP SIZE 0.12195E-05
CONTROLLING VARIABLE CO
RELATIVE ERROR 0.27813E-05
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/CM**2/SEC)	RATE CONSTANT (CGS UNITS)	
CH4	4.38649E-07	3.61137E-02	-4.42251E-03	1	-1.26010E+07	4.08588E+01	
CH3	2.04270E-08	1.68174E-03	8.57471E-04	2	-1.59549E+01	1.14917E+05	
H	2.83059E-10	2.33041E-05	2.19723E-05	3	-2.98447E+03	2.12473E+15	
O2	2.25360E-06	1.85538E-01	-4.37765E-03	4	5.07536E+01	1.10140E+08	
H2O	3.12822E-09	2.57545E-04	1.34470E-04	5	2.95077E+04	7.50000E+10	
CO	2.39250E-08	1.96473E-03	1.37533E-03	6	2.25333E+03	2.25502E+12	
CO2	1.69376E-10	1.39447E-05	1.13334E-05	7	1.50317E+03	1.38896E+12	
O	2.89766E-10	2.38562E-05	1.88218E-05	8	3.41728E+04	1.30162E+13	
CH2O	1.19976E-07	9.87759E-03	2.15630E-03	9	5.02576E+03	1.10823E+12	
OH	7.17839E-10	5.90992E-05	4.02146E-05	10	3.25090E+01	1.72745E+12	
H2	8.16594E-09	6.72297E-04	4.41195E-04	11	1.31713E+02	4.78735E+12	
H2O	1.68632E-07	1.38809E-02	4.85094E-03	12	4.61082E+01	3.14299E+11	
HCO	3.06641E-10	2.52455E-05	2.20777E-05	13	9.01164E+02	1.00000E+13	
H2O2	5.09452E-12	5.01758E-07	1.00850E-05	14	1.62525E+03	5.59998E+12	
N2	9.10809E-06	7.49863E-01	0.	15	7.14074E+03	9.70158E+12	
				16	3.27392E+03	1.10188E+13	
				17	5.69499E+06	7.49934E+12	
				18	8.62170E+00	4.58293E+12	
				19	4.63598E+01	6.24945E+13	
				20	5.64838E+03	2.08857E+11	
				21	5.14216E+03	8.70672E+11	
				22	1.50538E+02	1.80000E+12	
				23	5.29744E+02	7.00000E+13	
				24	4.64722E+01	6.00000E+12	
				25	1.14937E+02	6.00000E+12	
				26	1.41919E+02	2.18489E+11	
				27	1.07621E-01	2.3372E+15	
				28	-1.19477E-03	1.79765E+01	
				29	1.10006E+02	3.11420E+11	
MIXTURE MOLECULAR WEIGHT	28.16166		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/CM**2/SEC)	-2.26552E+09	MASS FRACTION SUM	0.9999966	
VARIABLE	DERIVATIVE (ATM)	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.21270E+07	0.93730E+00	0.30185E-08	CO2	0.33133E-01	0.13881E-07	0.49584E-05
RHO	-0.52240E+00	-0.22120E-06	0.11550E-07	O	0.49173E-01	0.10842E-07	0.94490E-05
T	0.23762E+07	0.10041E+01	0.24752E-07	CH2O	0.63038E+01	0.26795E-05	0.26765E-06
CH4	-0.12929E+02	-0.54661E-05	0.14186E-06	CH	0.11757E+00	0.48744E-07	0.18138E-04
CH3	0.25058E+01	0.10566E-05	0.91847E-06	42	0.12999E+01	0.54225E-06	0.25231E-05
H	0.64235E-01	0.25643E-07	0.41097E-04	420	0.14182E+02	0.59900E-05	0.59519E-05
O2	-0.12798E+02	-0.54106E-05	0.26448E-07	420	0.54543E-01	0.26690E-07	0.26756E-04
H2O	0.39312E+00	0.16840E-06	0.74604E-05	4202	0.29483E-02	0.79733E-09	0.44789E-03
CO	0.40207E+01	0.16894E-05	0.27813E-05	N2	0.	-0.	0.

TIME 2.54109E-04 SEC AREA 1.29688E+03 SQ CM AXIAL POSITION 4.00002E+01 CM

FLOW PROPERTIES

PRESSURE 1.73213
 VELOCITY 157347.14
 DENSITY 2.79004E-04
 TEMPERATURE (DEG K) 2079.27
 MASS FLOW RATE (GM/SEC) 5.69335E+04
 ENTRAPY (KCAL/GM/DEG K) 2.2635
 MACH NUMBER 1.7533
 GAMMA 1.2804

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 47
 AVERAGE STEP SIZE 0.68488E-06
 CONTROLLING VARIABLE CH4
 RELATIVE ERROR 0.22026E-04
 PREDICTOR ITERATIONS 3

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/CM**2/SEC)	RATE CONSTANT (CGS UNITS)	
CH4	2.19812E-08	2.16517E-03	-1.36697E-02	1	-7.90308E+04	5.66946E+03	
CH3	5.81446E-08	5.72729E-03	-1.82969E-02	2	-8.40127E+01	2.38854E+06	
H	2.04262E-08	2.01220E-03	3.72766E-03	3	-2.54021E+04	2.12538E+15	
O2	1.36024E-06	1.33985E-01	-6.46677E-02	4	4.77091E+03	7.94604E+08	
H2O	2.87405E-09	2.83097E-04	-9.68128E-04	5	7.62017E+04	7.50000E+10	
CO	3.48962E-07	3.43336E-02	4.25027E-02	6	1.51854E+04	3.96792E+12	
CO2	1.61630E-08	1.59207E-03	5.66453E-03	7	1.17258E+04	2.15788E+12	
O	2.35533E-08	2.32130E-03	1.26190E-02	8	2.27811E+05	1.72659E+13	
CH2O	4.34411E-08	4.28293E-03	-1.64855E-02	9	7.09275E+05	2.41898E+12	
OH	3.52731E-08	5.44445E-03	1.84423E-02	10	2.44047E+04	2.76200E+12	
H2	5.41490E-08	6.32070E-03	-1.54267E-03	11	1.30504E+05	6.11172E+12	
H2O	7.04358E-07	6.93799E-02	6.15599E-02	12	8.08437E+04	3.29716E+11	
HCO	3.87918E-09	3.52103E-04	-7.15077E-04	13	3.34451E+05	1.00000E+13	
H2O2	7.10913E-12	7.00256E-07	9.58076E-06	14	7.02792E+04	6.1285E+12	
N2	7.42707E-06	7.41770E-01	0.	15	3.56450E+05	1.15485E+13	
				16	1.95703E+05	1.46720E+13	
				17	9.63914E+03	8.20782E+12	
				18	1.38150E+04	5.01589E+12	
				19	6.96298E+04	6.3985E+13	
				20	4.54890E+05	8.99223E+11	
				21	8.35426E+04	1.23415E+12	
				22	1.90965E+02	1.00000E+12	
				23	5.27773E+04	7.00000E+13	
				24	5.21020E+03	6.00000E+12	
				25	1.22240E+04	6.00000E+12	
				26	6.66030E+01	1.3075E+12	
				27	7.38230E+02	1.77212E+15	
				28	-3.76232E-01	4.41533E+03	
				29	-2.92747E+04	7.17404E+11	

MIXTURE MOLECULAR WEIGHT 27.48216 TOTAL ENERGY EXCHANGE RATE -5.17806E+10 MASS FRACTION SUM 1.00000054
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.26436E+09	-0.12834E+02	0.86516E-07	CO2	0.23887E+02	0.11511E-05	0.19943E-05
RHO	-0.53647E+01	-0.26128E-06	0.73088E-07	O	0.45229E+02	0.21985E-05	0.74691E-04
T	0.47344E+08	0.23020E+01	0.24559E-06	CH2O	-0.59087E+02	-0.28876E-05	0.94870E-05
CH4	-0.48995E+02	-0.24160E-05	0.22026E-04	OH	0.66100E+02	0.33153E-05	0.43277E-04
CH3	-0.65579E+02	-0.31588E-05	0.30385E-05	H2	-0.55272E+01	-0.25374E-06	0.64559E-06
H	0.20529E+02	0.99778E-06	0.73094E-05	H2O	0.22064E+03	0.10696E-04	0.50794E-06
O2	-0.23178E+03	-0.11255E-04	0.18244E-06	HCO	-0.25630E+01	-0.11532E-06	0.92039E-04
H2O2	-0.34699E+01	-0.16909E-06	0.65731E-05	H2O2	0.34698E-01	0.11052E-04	0.10714E-02
CO	0.15234E+03	0.74266E-05	0.11337E-05	N2	0.	-0.	0.

METHANE-AIR COMBUSTION

(ASSIGNED PRESSURE)

CASE 7

REACTION NUMBER	REACTION	REACTION RATE VARIABLES		ACTIVATION ENERGY
		A	N	
1	CH4 + O2 = CH3 + OH	3.80000E+14	0.	103000.00
2	CH4 + O2 = CH3 + OH2	1.20000E+13	0.	63900.00
3	H + O2 = HO2	1.59000E+15	0.	-1000.00
4	CO + O2 = CO2	1.50000E+13	0.	41000.00
5	CH3 + O2 = CH2O + OH	7.50000E+10	0.	0.
6	H + CH4 = CH3 + H2	5.70000E+13	0.	11800.00
7	O + CH4 = CH3 + OH	2.00000E+13	0.	9200.00
8	OH + CH4 = CH3 + H2O	7.20000E+13	0.	5900.00
9	H + O2 = OH + O	1.25000E+14	0.	16300.00
10	O + H2 = OH + H	2.96000E+13	0.	9800.00
11	H2 + O2 = H2O + O	2.10000E+13	0.	5100.00
12	CO + O2 = CO2	4.20000E+11	0.	1000.00
13	CH3 + O = CH2O + H	1.90000E+13	0.	0.
14	CH2O + H = HCO + H2	1.00000E+13	0.	2000.00
15	CH2O + O = HCO + OH	7.30000E+10	0.7000	1000.00
16	CH2O + O = HCO + OH	4.00000E+11	0.6000	4000.00
17	HCO + O = CO + OH	1.80000E+11	0.5000	0.
18	HCO + O2 = CO + H2O	1.10000E+11	0.5000	0.
19	HCO + H = CO + H2	1.50000E+12	0.5000	0.
20	H + HCO = H2 + CO	2.00000E+13	0.5000	28600.00
21	HCO + O2 = CO + OH2	1.30000E+11	0.5000	5400.00
22	H + OH2 = OH + H2	1.80000E+12	0.	0.
23	H + OH2 = OH + H2	7.00000E+13	0.	0.
24	O + H2 = OH + H	6.00000E+12	0.	0.
25	OH + H2 = H2O + H	5.00000E+12	0.	0.
26	H + H2O2 = H2O + OH	1.17000E+17	0.	45500.00
27	H + O2 = OH + O	7.50000E+23	-2.6000	0.
28	H + O2 = OH + O	2.75000E+19	-1.0000	118700.00
29	O + H2O = OH + O	5.75000E+13	0.	18000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

MICH4	+ 31 =	5.00000	M(O2	+ 31 =	2.00000	M(H2	+261 =	0.78000	M(O2	+271 =	1.60000
MICO	+ 31 =	2.00000	M(O2	+ 31 =	7.50000	M(H2	+ 31 =	5.00000	M(H2O	+ 31 =	32.50000
M(H2O	+261 =	6.00000	M(H2O	+271 =	20.00000	M(H2O2	+261 =	5.60000	M(H2	+ 31 =	2.00000
M(H2	+271 =	1.50000									

INTEGRATION CONTROLS

MINIMUM STEP SIZE 0.10000E-03 CM

MAXIMUM STEP SIZE 0.20000E+00 CM

INITIAL STEP SIZE 0.20000E-01 CM

MAXIMUM RELATIVE ERROR 0.00010

** ASSIGNED VARIABLE PROFILE **

THE PRESSURE IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE

STATION	AXIAL DISTANCE (CM)	PRESSURE (ATM)
1	0.	1.73303E+00
2	5.00000E+00	1.73132E+00
3	1.00000E+01	1.73598E+00
4	1.50000E+01	1.74540E+00
5	2.00000E+01	1.75313E+00
6	2.50000E+01	1.78070E+00
7	2.75000E+01	1.80180E+00
8	3.00000E+01	1.82537E+00
9	3.25000E+01	1.87180E+00
10	3.50000E+01	1.99243E+00
11	3.55000E+01	2.04700E+00
12	3.60000E+01	2.14350E+00
13	3.65000E+01	2.36787E+00
14	3.70000E+01	3.10027E+00

THE FOLLOWING SPECIES WILL BE NEGLECTED FROM ALL ERROR CONSIDERATIONS

CO2	H	O4	HO2	O
		4202	CH3	

** INITIAL CONDITIONS **

TIME	0.	SEC	AREA	1.00000E-01	SQ M	AXIAL POSITION	0.	M
FLOW PROPERTIES					INTEGRATION INDICATORS			
PRESSURE	(V/M**2)	1.75292E+05	STEPS FROM LAST PRINT			0		
VELOCITY	(M/SEC)	1.57413E+03	AVERAGE STEP SIZE			0.		
DENSITY	(KG/M**3)	3.61559E-01	CONTROLLING VARIABLE					
TEMPERATURE	(DEG K)	1.64500E+03						
MASS FLOW RATE	(KG/SEC)	5.69139E+01						
ENTROPY	(J/MOL/DEG K)	8.91515E+03	RELATIVE ERROR			0.		
MACH NUMBER		2.00000E+00	PREDICTOR ITERATIONS			0		
GAMMA		1.27772E+00						

CHEMICAL PROPERTIES						
SPECIES	CONCENTRATION (MOLES/M**3)	MOL FRACTION	NET SPECIES PRODUCTION RATE (MOLE/M**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-M**3/KG**2/SEC)	RATE CONSTANT (CGS UNITS)
CH4	5.3752E-04	4.7680E-02	-5.08397E-03	1	3.83546E-02	7.96181E+00
CH3	0.	0.	5.08397E-03	2	5.31069E-04	4.26588E+00
H	0.	0.	5.01454E-03	3	0.	2.15901E+15
O2	2.55141E-03	1.99072E-01	-6.95166E-05	4	0.	5.71435E+07
H2O	0.	0.	6.94238E-05	5	0.	7.50000E+10
CO	0.	0.	0.	6	0.	1.46697E+12
CO2	0.	0.	0.	7	0.	1.19880E+12
O	0.	0.	1.85518E-07	8	0.	1.18434E+13
CH2O	0.	0.	0.	9	0.	8.33770E+11
OH	0.	0.	0.	10	0.	1.76705E+12
H2	0.	0.	0.	11	0.	4.41213E+12
H2O	0.	0.	0.	12	0.	3.49309E+11
HCO	0.	0.	0.	13	0.	1.40000E+13
H2O2	0.	0.	0.	14	0.	5.42358E+12
N2	7.62725E-03	7.01160E-01	0.	15	0.	9.19511E+12
				16	0.	1.00075E+13
				17	0.	7.30055E+12
				18	0.	4.46145E+12
				19	0.	6.18379E+13
				20	0.	1.18648E+11
				21	0.	7.77419E+11
				22	0.	1.40000E+12
				23	0.	7.00000E+13
				24	0.	6.00000E+12
				25	0.	6.00000E+12
				26	0.	1.05485E+11
				27	0.	3.25857E+13
				28	7.09957E-07	2.3818E+00
				29	0.	2.33475E+11

MIXTURE MOLECULAR WEIGHT 28.21038 TOTAL ENERGY EXCHANGE RATE 1.69508E+07 MASS FRACTION SUM 0.9999999

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.76732E+01	0.	0.	CO2	0.	0.	0.
RHO	9.76108E-07	0.	0.	O	3.32514E-11	0.	0.
T	0.59452E-01	0.	0.	CH2O	0.	0.	0.
CH4	-0.89327E-07	0.	0.	OH	0.	0.	0.
CH3	0.89327E-07	0.	0.	H2	0.	0.	0.
H	0.88108E-07	0.	0.	H2O	0.	0.	0.
O2	-0.12214E-08	0.	0.	H2O2	0.	0.	0.
H2O	0.122198E-08	0.	0.	N2	0.	0.	0.
CO	0.	0.	0.				

TIME 1.91107E-04 SEC AREA 1.00009E-01 SQ M AXIAL POSITION 3.00000E-01 M

FLOW PROPERTIES

PRESSURE	1.84956E+05
(N/M**2)	
VELOCITY	1.55715E+03
(M/SEC)	
DENSITY	3.65468E-01
(KG/M**3)	
TEMPERATURE	1.71605E+03
(DEG K)	
MASS FLOW RATE	5.69139E+01
(KG/SEC)	
ENTROPY	8.98216E+03
(J/JUL/KG/DEG K)	
MACH NUMBER	1.93769E+00
GAMMA	1.27611E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	51
AVERAGE STEP SIZE	0.19860E+00
CONTROLLING VARIABLE	HCO
RELATIVE ERROR	0.21320E-04
PREDICTOR ITERATIONS	0

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CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/M**3)	MOL FRACTION	NET SPECIES PRODUCTION RATE (MOLE/M**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-M**3/KG**2/SEC)	RATE CONSTANT (CGS UNITS)
CH4	3.44622E-04	4.20144E-02	-2.18510E+00	1	3.3554E-02	2.39815E+01
CH3	9.98045E-06	7.89934E-04	3.05291E-01	2	-1.60425E-03	3.47491E+04
H	7.68076E-03	5.92526E-06	4.38061E-03	3	-8.06005E-01	2.13183E+15
O2	2.48300E-03	1.91549E-01	-2.11269E+00	4	1.35045E-02	9.60563E+07
H2O	1.12407E-06	8.67157E-05	4.40713E-02	5	1.39152E+01	7.50000E+10
CO	7.56270E-06	5.63418E-04	3.54750E-01	6	6.60000E-01	2.16735E+12
CO2	4.73686E-08	3.5606E-06	2.49700E-03	7	5.84238E-01	1.34595E+12
O	1.0651E-07	8.21979E-06	4.60052E-03	8	1.50314E+01	1.27825E+13
CH2O	3.24577E-05	6.16113E-03	1.51720E+00	9	1.49652E+00	1.74955E+12
OH	2.92710E-07	2.25308E-05	1.03975E-02	10	3.64037E-03	1.47187E+12
H2	2.90130E-06	2.23819E-04	1.21151E-01	11	1.57960E-02	4.70655E+12
H2O	9.91364E-05	7.66478E-03	2.24058E+00	12	5.19013E-03	3.13252E+11
HCO	7.82593E-08	6.03725E-06	4.35799E-03	13	1.51273E-01	1.00000E+13
H2O2	3.81377E-10	6.79331E-08	1.43422E-04	14	2.63750E-01	5.6273E+12
N2	9.73155E-03	7.0717E-01	0.	15	1.73331E+00	9.4210E+12
				16	7.10303E-01	1.7983E+13
				17	4.55514E-04	7.45655E+12
				18	7.31505E-04	4.55578E+12
				19	2.79637E-03	6.1379E+13
				20	1.43367E+00	1.8762E+11
				21	1.23696E+00	8.90244E+11
				22	1.70273E-02	1.00000E+12
				23	4.52478E-02	7.00000E+13
				24	5.37644E-03	6.00000E+12
				25	1.47074E-02	5.00000E+12
				26	1.59545E-02	1.7711E+11
				27	1.03757E-05	2.41931E+13
				28	2.5897E-06	1.22363E+01
				29	2.02842E-02	2.43253E+11

MIXTURE MOLECULAR WEIGHT 28.19374 TOTAL ENERGY EXCHANGE RATE -4.09806E+09 MASS FRACTION SUM 0.9999969
(JJULE-M**3/KG**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.21174E+03	-0.26723E+02	0.22852E-07	CO2	0.43377E-07	0.54972E-03	0.66147E-03
RHO	0.79464E-06	0.36227E-07	0.57501E-07	O	0.80842E-07	0.10218E-07	0.87874E-05
T	0.95310E+01	0.12070E+01	0.51835E-07	CH2O	0.26660E-04	0.33933E-03	0.30313E-06
CH4	-0.38396E-04	-0.48695E-05	0.16567E-05	O4	0.18200E-06	0.22660E-07	0.71072E-05
CH3	0.53820E-05	0.67855E-06	0.25000E-05	H2	0.21290E-05	0.26750E-06	0.44469E-05
H	0.76976E-07	0.90339E-08	0.24828E-04	H2O	0.39373E-04	0.49904E-05	0.10232E-05
O2	-0.37124E-04	-0.47085E-05	0.34525E-07	HCO	0.76754E-07	0.92979E-07	0.21370E-04
HO2	0.77443E-06	0.98535E-07	0.15466E-06	H2O2	0.25202E-08	0.15237E-09	0.31923E-03
CO	0.62336E-05	0.78280E-06	0.50641E-05	N2	0.	-0.	0.

TIME 2.33390E-04 SEC AREA 1.00160E-01 SQ M AXIAL POSITION 3.65000E-01 M

FLOW PROPERTIES

PRESSURE 2.39954E+05
(N/M**2)
VELOCITY 1.46043E+03
(M/SEC)
DENSITY 3.89082E-01
(KG/M**3)
TEMPERATURE 2.05581E+03
(DEG K)
MASS FLOW RATE 5.69139E+01
(KG/SEC)
ENTROPY 9.30386E+03
(JJULE/KG/DEG K)
MACH NUMBER 1.64671E+00
GAMMA 1.27631E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 32
AVERAGE STEP SIZE 0.47137E-01
CONTROLLING VARIABLE HCO
RELATIVE ERROR 0.69549E-04
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/M**3)	MOLF FRACTION	NET SPECIES PRODUCTION RATE (MOLE/M**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-M**3/KG**2/SEC)	RATE CONSTANT (CDS UNITS)
CH4	1.27394E-04	9.08129E-03	-5.29101E+01	1	-5.29305E+01	4.26614E+03
CH3	1.26807E-04	9.03939E-03	5.84308E+00	2	-1.91961E-01	2.00716E+06
H	1.27314E-05	9.07554E-04	6.06024E+00	3	-4.40838E+01	2.33098E+15
O2	2.15298E-03	1.53475E-01	-8.56467E+01	4	2.89188E+00	7.00620E+08
HO2	5.98892E-06	4.76919E-04	-1.23559E+00	5	1.35257E+02	7.50000E+10
CO	2.90293E-04	2.06935E-02	6.93123E+01	6	3.13736E+01	3.84071E+12
CO2	5.19770E-06	4.41801E-04	3.07359E+00	7	1.80851E+01	2.10375E+12
O	1.10367E-05	7.86751E-04	6.46573E+00	8	3.53170E+02	1.69869E+13
CH2O	1.30980E-04	9.33686E-03	-2.57899E+01	9	4.00099E+02	2.31252E+12
OH	2.77538E-05	1.97843E-03	1.54780E+01	10	1.01123E+01	2.68826E+12
H2	7.51074E-05	5.35401E-03	1.07797E+01	11	4.46193E+01	6.02625E+12
H2O	5.96119E-04	4.46227E-02	1.01577E+02	12	1.74113E+01	3.28807E+11
HCO	4.73507E-06	3.37538E-04	4.70935E-01	13	1.75632E+02	1.90000E+13
H2O2	4.14200E-09	2.95133E-07	1.98843E-03	14	6.74820E+01	6.12891E+12
N2	1.03601E-02	7.38518E-01	0.	15	2.74305E+02	1.14256E+13
				16	1.39482E+02	1.46089E+13
				17	2.81740E+00	8.16139E+12
				18	4.32964E+00	4.98752E+12
				19	2.70834E+01	6.80116E+13
				20	3.62523E+02	8.26240E+11
				21	8.14050E+01	1.20900E+12
				22	4.26453E-01	1.40000E+12
				23	3.52544E+01	7.00000E+13
				24	2.61612E+00	6.00000E+12
				25	6.57435E+00	6.00000E+12
				26	4.13331E-01	1.70279E+12
				27	1.47059E-01	1.82517E+15
				28	-5.40082E-03	3.21782E+03
				29	1.14966E+01	7.16485E+11

MIXTURE MOLECULAR WEIGHT 27.73562 TOTAL ENERGY EXCHANGE RATE -1.46076E+11 MASS FRACTION SUM 1.0000006
(JJULE-M**3/KG**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.19448E+05	-0.39447E+03	0.66301E-06	CO2	0.54091E-04	0.10803E-05	0.60749E-04
RHO	0.76145E-04	0.15351E-05	0.37566E-06	O	0.11391E-03	0.21414E-05	0.11797E-03
T	0.44009E+03	0.10004E+02	0.12639E-05	CH2O	-0.45395E-03	-0.93013E-05	0.39734E-05
CH4	-0.73114E-03	-0.19526E-04	0.81814E-05	O4	0.27239E-03	0.15009E-07	0.88390E-04
CH3	0.10263E-03	0.25062E-05	0.24050E-04	H2	0.18971E-03	0.39939E-07	0.59551E-05
H	0.10665E-03	0.20898E-05	0.55839E-04	H2O	0.17894E-02	0.15887E-07	0.30170E-05
O2	-0.15673E-02	-0.30844E-04	0.18514E-05	HCO	0.82879E-05	0.25557E-06	0.69549E-04
HO2	-0.21762E-04	-0.42030E-06	0.22533E-04	H2O2	0.34958E-07	-0.18635E-09	0.34491E-03
CO	0.12198E-02	0.24986E-04	0.89456E-05	N2	0.	-0.	0.

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

H2-O2 LOW TEMPERATURE REACTION AT CONSTANT VOLUME (ADJUSTED RATES) CASE 8

REACTION NUMBER	REACTION				REACTION RATE VARIABLES		ACTIVATION ENERGY
	A	N					
1	H2	+ O2	= H	+ HO2	1.00000E+14	0.	67000.00
2	H2	+ OH	= H2O	+ H	2.10000E+13	0.	51000.00
3	H	+ O2	= OH	+ O	1.25000E+14	0.	163000.00
4	O	+ H2	= OH	+ H	2.96000E+13	0.	98000.00
5	H	+ O2	= HO2	+ H	8.50000E+14	0.	-10000.00
6	H	+ HO2	= OH	+ O2	7.00000E+13	0.	0.
7	H	+ H2O2	= OH	+ OH	1.17000E+17	0.	45500.00
8	HO2	+ H2O2	= H2O2	+ O2	1.00000E+12	0.	0.
9	HO2	+ H2	= H2O2	+ H	8.50000E+12	0.	24000.00
10	H	+ H2O2	= H2O	+ OH	3.18000E+14	0.	9000.00
11	OH	+ H2O2	= H2O	+ HO2	1.00000E+13	0.	18000.00
12	O	+ H2O	= OH	+ OH	5.75000E+13	0.	18000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2 , 5) = 5.00000 M(H2 , 7) = 2.30000 M(O2 , 5) = 2.00000 M(O2 , 7) = 0.78000
M(H2O , 5) = 32.50000 M(H2O , 7) = 6.00000 M(H2O2 , 5) = 5.60000

INTEGRATION CONTROLS

MINIMUM STEP SIZE 0.50000E-04 SEC

MAXIMUM STEP SIZE 0.10000E+00 SEC

INITIAL STEP SIZE 0.15000E+00 SEC

MAXIMUM RELATIVE ERROR 0.00030

** ASSIGNED VARIABLE PROFILE **

THIS IS A V=0 PROBLEM - AN ASSIGNED VARIABLE IS NOT REQUIRED

THE FOLLOWING SPECIES WILL BE NEGLECTED FROM ALL ERROR CONSIDERATIONS

O H OH HO2

THE VOLUME (DENSITY) WILL BE HELD CONSTANT FOR THIS CASE

THE TEMPERATURE WILL BE HELD CONSTANT FOR THIS CASE

** INITIAL CONDITIONS **

TIME 0. SEC AREA 1.00000E+00 SQ CM AXIAL POSITION 0. CM

FLOW PROPERTIES

PRESSURE 0.65789
(ATM)
VELOCITY 0.
(CM/SEC)
DENSITY 6.44320E-05
(GM/CM**3)
TEMPERATURE 773.15
(DEC K)
MASS FLOW RATE 0.
(GM/SEC)
ENTRPHY 6.7684
(CAL/GM/DEC K)
MACH NUMBER 0.
GAMMA 1.3810

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	2.79028E-01	8.60000E-01	-1.48936E-16	1	3.58755E-08	1.15030E-05
O2	7.20972E-01	1.40000E-01	-1.48936E-16	2	0.	7.59590E+11
H	0.	0.	1.48936E-16	3	0.	3.08543E+09
HO2	0.	0.	1.48936E-16	4	0.	5.02437E+10
OH	0.	0.	0.	5	0.	1.62965E+15
H2O	0.	0.	0.	6	0.	7.00000E+13
O	0.	0.	0.	7	0.	1.60878E+04
H2O2	0.	0.	0.	8	0.	1.00000E+12
				9	0.	1.39711E+06
				10	0.	9.08566E+11
				11	0.	3.09875E+12
				12	0.	4.69383E+08

MIXTURE MOLECULAR WEIGHT 6.21325 TOTAL ENERGY EXCHANGE RATE 2.04835E-03 MASS FRACTION SUM 1.00000000
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.	0.	0.	H	0.23115E-11	0.	0.
RHO	0.	0.	0.	H02	0.23115E-11	0.	0.
T	0.	0.	0.	D	0.	0.	0.
H2	-0.23115E-11	0.	0.	H20	0.	0.	0.
O2	-0.23115E-11	0.	0.	D	0.	0.	0.
				H202	0.	0.	0.

TIME 3.00000E-01 SEC AREA 1.00000E+00 SQ CM AXIAL POSITION -0. CM

FLOW PROPERTIES

PRESSURE 0.65789
(ATM)
VELOCITY 0.
(CM/SEC)
DENSITY 6.44320E-05
(GM/CM**3)
TEMPERATURE 773.15
(DEG K)
MASS FLOW RATE 0.
(GM/SEC)
ENTROPY 6.7684
(CAL/GM/DEG K)
MACH NUMBER 0.
GAMMA 1.3810

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 2
AVERAGE STEP SIZE 0.15000E+00
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	2.79028E-01	8.60000E-01	-2.14987E-15	1	3.58755E-08	1.15030E-05
O2	7.20972E-01	1.40000E-01	-2.14987E-15	2	7.28558E-08	7.59590E-11
H	2.68006E-16	1.65202E-15	1.48906E-16	3	1.84851E-08	3.08543E-09
H02	5.66724E-11	1.25512E-11	4.51396E-16	4	1.84852E-08	5.02437E+10
OH	1.17851E-17	4.30591E-18	1.32340E-22	5	4.63503E-07	1.62965E+15
H2O	1.14108E-11	3.93572E-12	3.02459E-15	6	3.75977E-14	7.00000E+13
O	4.25271E-17	1.65151E-17	-2.98612E-22	7	1.79427E-08	1.60878E+04
H202	1.12929E-10	2.06284E-11	1.54726E-15	8	3.59439E-12	1.00000E+12
				9	3.90640E-07	1.39711E+06
				10	8.02049E-16	9.08566E+11
				11	7.10905E-18	3.09875E+12
				12	7.86538E-22	4.69383E+08

MIXTURE MOLECULAR WEIGHT 6.21325 TOTAL ENERGY EXCHANGE RATE -1.39228E-02 MASS FRACTION SUM 0.99999998
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	0.	0.	0.	H	0.23111E-11	0.	0.
RHO	0.	0.	0.	H02	0.70053E-11	0.	0.
T	0.	0.	0.	D	0.23540E-17	0.	0.
H2	-0.33367E-10	0.	0.	H20	0.45942E-11	0.	0.
O2	-0.33367E-10	0.	0.	O	-0.45345E-17	0.	0.
				H202	0.24014E-10	0.	0.

TIME 5.50000E+01 SEC AREA 1.00000E+00 SQ CM AXIAL POSITION -0. CM

FLOW PROPERTIES

PRESSURE 0.64423
(ATM)
VELOCITY -0.
(CM/SEC)
DENSITY 6.44320E-05
(GM/CM**3)
TEMPERATURE 773.15
(DEG K)
MASS FLOW RATE -0.
(GM/SEC)
ENTROPY 6.7269
(CAL/GM/DEG K)
MACH NUMBER 0.
GAMMA 1.3756

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 34
AVERAGE STEP SIZE 0.14853E+00
CONTROLLING VARIABLE H2
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0
ELIMINATED SPECIES H202

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
H2	2.65937E-01	8.7039E-01	-1.29232E-08	1	-1.19937E-04	1.15030E-05
O2	5.13941E-01	1.1754E-01	-5.46592E-09	2	2.84216E+00	7.59590E+11
H	1.47444E-09	9.18144E-09	-6.75755E-12	3	8.66045E-02	3.08543E-09
H02	3.50054E-05	6.92209E-06	5.93480E-12	4	8.65659E-02	5.02437E+10
OH	4.82617E-10	1.50057E-10	1.70456E-12	5	2.66114E+00	1.62965E+15
H2O	1.13513E-01	3.9828E-02	1.29272E-08	6	1.11706E-01	7.00000E+13
O	2.08756E-10	8.18691E-11	1.94819E-19	7	1.10375E+00	1.60878E+04
H202	5.52167E-03	1.11782E-03	-4.44899E-12	8	1.19012E+00	1.00000E+12
				9	1.84403E-01	1.39711E+06
				10	2.55044E-01	9.08566E+11
				11	1.67694E-02	3.09875E+12
				12	3.96216E-05	4.69383E+08

MIXTURE MOLECULAR WEIGHT 6.34507 TOTAL ENERGY EXCHANGE RATE -1.80008E+05 MASS FRACTION SUM 0.99999548
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.	-0.	0.	H	-0.10488E-06	-0.33141E-12	0.88715E-05
RHO	0.	0.	0.	H02	0.92110E-07	0.99000E-10	0.13979E-05
T	0.	0.	0.	OH	0.26457E-07	0.78008E-14	0.68737E-06
H2	-0.20057E-03	-0.20072E-04	0.	H2O	0.20063E-03	0.20078E-04	0.
O2	-0.10035E-03	-0.10033E-04	0.	O	0.30236E-14	-0.78279E-14	0.88785E-05
				H2O2	-0.69049E-07	-0.61655E-08	0.42873E-07

TIME 1.20000E+02 SEC AREA 1.00000E+00 SQ CM AXIAL POSITION -0. CM

FLOW PROPERTIES

PRESSURE 0.61855
(ATM)
VELOCITY -0.
(CM/SEC)
DENSITY 6.44320E-05
(GM/CM**3)
TEMPERATURE 773.15
(DEG K)
MASS FLOW RATE -0.
(GM/SEC)
ENTROPY 6.6034
(CAL/GM/DEG K)
MACH NUMBER 0.
GAMMA 1.3657

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 101
AVERAGE STEP SIZE 0.14852E+00
CONTROLLING VARIABLE H2O2
RELATIVE ERROR 0.25645E-10
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CDS UNITS)
H2	2.40550E-01	7.88565E-01	-1.17207E-08	1	-1.14644E-04	1.15030E-05
O2	4.13001E-01	8.52987E-02	-5.84203E-09	2	2.60492E+00	7.59590E+11
H	1.46904E-09	9.63131E-09	-1.79357E-13	3	5.80421E-02	3.08543E+09
H02	3.45437E-05	6.91595E-06	3.37780E-12	4	5.79565E-02	5.02437E+10
OH	4.89618E-10	1.90252E-10	3.82663E-15	5	2.44450E+00	1.62965E+15
H2O	3.40905E-01	1.25062E-01	1.17608E-08	6	1.06766E-01	7.06000E+13
O	1.54663E-10	6.38828E-11	-1.11057E-15	7	1.03767E+00	1.60878E+04
H2O2	5.49669E-03	1.06793E-03	-4.17583E-11	8	1.09521E+00	1.00000E+12
				9	1.60490E-01	1.39711E+06
				10	2.13986E-01	9.08566E+11
				11	1.41050E-02	3.09875E+12
				12	8.58655E-05	4.69983E+08

MIXTURE MOLECULAR WEIGHT 6.60846 TOTAL ENERGY EXCHANGE RATE -1.63402E+05 MASS FRACTION SUM 0.99998793
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.	-0.	0.	H	-3.27837E-08	-0.63249E-12	0.34664E-06
RHO	0.	0.	0.	H02	3.52424E-07	0.13013E-10	0.10178E-07
T	0.	0.	0.	OH	0.59390E-10	0.25904E-14	0.72024E-07
H2	-0.18191E-03	-0.43891E-07	0.	H2O	0.18253E-03	0.44041E-07	0.
O2	-0.90670E-04	-0.21877E-07	0.57412E-12	O	-3.17236E-10	-0.41662E-14	0.34317E-06
				H2O2	-0.64810E-06	-0.15657E-09	0.25645E-10

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

01 UNIT05, EOF.

REC= 00000 FIL= 00002

HIGH TEMPERATURE AIR IONIZATION

CASE 9

REACTION NUMBER	REACTION					REACTION RATE VARIABLES			ACTIVATION ENERGY
	A	N				A	N		
1	N	+ O2	= NO	+ O		6.43000E+09	1.0000		6500.00
2	O	+ N2	= NO	+ N		1.36000E+14	0.		75400.00
3	N	+ O	= NO	+ M		6.40000E+16	-0.5000		0.
4	O	+ O	= O2	+ M		1.38000E+18	-1.0000		340.00
5	N	+ N	= N2	+ M		2.80000E+17	-0.7000		0.
6	NO	+ O	= NO2	+ M		9.40000E+14	0.		-1930.00
7	M	+ N2O	= N2	+ O2		5.00000E+14	0.		98000.00
8	O	+ N2O	= N2	+ O2		6.30000E+14	0.		26700.00
9	NO+	+ E	= N	+ O		1.45000E+21	-1.5000		0.
10	O+	+ E	= O	+ M		2.00000E+26	-2.5000		0.
11	O2	+ E	= O2-	+ M		1.52000E+21	-1.0000		1190.00
12	O2	+ O-	= O2-	+ O		6.00000E+12	0.		0.

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M1N	,10) =	0.03000	M1O2	,10) =	4.50000	M1NO	,10) =	50.00000	M1O	,10) =	0.03000
M1N2	,6) =	1.55000	M1N2	,11) =	0.00002	M1N2O	,3) =	2.25000			

INTEGRATION CONTROLS

MINIMUM STEP SIZE 0.10000E-02 CM

MAXIMUM STEP SIZE 0.30000E+00 CM

INITIAL STEP SIZE 0.20000E-02 CM

MAXIMUM RELATIVE ERROR 0.00010

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

$$\text{AREA (CM**2)} = (0. \quad)X**3 + (0. \quad)X**2 + (0. \quad)X + (1.00000E+03)$$

THE FOLLOWING SPECIES WILL BE NEGLECTED FROM ALL ERROR CONSIDERATIONS

E O- NO+ O+ O2-

** INITIAL CONDITIONS **

TIME 0. SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 0. CM

FLOW PROPERTIES

PRESSURE 1.58030
(ATM)
VELOCITY 47002.00
(CM/SEC)
DENSITY 1.22557E-04
(GM/CM**3)
TEMPERATURE 4820.00
(DEG K)
MASS FLOW RATE 5.76045E+03
(GM/SEC)
ENTROPY 2.3909
(CAL/GM/DEG K)
MACH NUMBER 0.3535
GAMMA 1.2723

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.
CONTROLLING VARIABLE
RELATIVE ERROR 0.
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLL FRACTION	NET SPECIES PRODUCTION RATE (MDLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
N	0.	0.	1.57461E-05	1	0.	1.1387E+13
O2	3.90048E-07	2.09500E-01	-9.46229E-02	2	0.	5.18479E+10
NO	0.	0.	0.	3	0.	9.21842E+14
O	0.	0.	1.80102E-01	4	-5.35802E+06	2.76322E+14
N2	3.35839E-06	7.90500E-01	-1.91514E-02	5	-5.24160E+02	4.74031E+14
NO2	0.	0.	0.	6	0.	1.14984E+15
N2O	0.	0.	1.91435E-02	7	0.	1.17251E+12
NO+	0.	0.	0.	8	-1.27451E+06	3.07884E+13
E	0.	0.	0.	9	0.	4.33309E+15
O+	0.	0.	0.	10	0.	1.23997E+17
O2-	0.	0.	0.	11	0.	2.78509E+17
O-	0.	0.	0.	12	0.	6.00000E+12
MIXTURE MOLECULAR WEIGHT		28.84765	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)		7.39254E+11	MASS FRACTION SUM 1.00000000

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.47607E+05	0.	0.	N2	-0.39246E-02	0.	0.
RHO	0.12466E-03	0.	0.	O	0.	0.	0.
T	-0.60657E+04	0.	0.	N2O	0.33233E-02	0.	0.
N	0.27335E-05	0.	0.	NO+	0.	0.	0.
O2	-0.17244E-01	0.	0.	E	0.	0.	0.
NO	0.	0.	0.	O+	0.	0.	0.
O	0.31265E-01	0.	0.	O2-	0.	0.	0.
				O-	0.	0.	0.

AA -0.33999E+00		BB 0.12931E+01		J(AREA)/D(IVAR) 0.		D2(AREA)/D(IVAR)2 0.		(1/AREA)*D(AREA)/D(IVAR)-AA 0.86999E+00	
OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J									
SPECIES	1 9	2 10	3 11	REACTION 4 12	5	6	7	8	
N	-0. 0.	0. 0.	-0. 0.	-0. 0.	0.15746E-04	0.	0.	-0.	
O2	-0. 0.	0. 0.	0. -0.	-0.80479E-01 -0.	-0.	0.	0.	-0.19144E-01	
NO	0. 0.	0. 0.	0. 0.	-0. 0.	-0.	-0.	0.	-0.	
O	0. 0.	-0. 0.	-0. 0.	0.16096E+00 0.	-0.	-0.	0.	0.19144E-01	
N2	0. 0.	-0. 0.	0. 0.	-0. 0.	-0.78731E-05	0.	0.	-0.19144E-01	
NO2	0. 0.	0. 0.	0. 0.	-0. 0.	-0.	0.	0.	-0.	
N2O	0. 0.	0. 0.	0. 0.	-0. 0.	-0.	0.	-0.	0.19144E-01	
NO+	0. -0.	0. 0.	0. 0.	-0. 0.	-0.	0.	0.	-0.	
E	0. -0.	0. -0.	0. -0.	-0. 0.	-0.	0.	0.	-0.	
O+	0. 0.	0. -0.	0. 0.	-0. 0.	-0.	0.	0.	-0.	
O2-	0. 0.	0. 0.	0. 0.	-0. 0.	-0.	0.	0.	-0.	
O-	0. 0.	0. 0.	0. 0.	-0. -0.	-0.	0.	0.	-0.	

TIME 4.29553E-07 SEC

AREA 1.00000E+03 SQ CM

AXIAL POSITION 2.00000E-02 CM

FLOW PROPERTIES

PRESSURE 1.68510
(ATM)
VELOCITY 46156.15
(CM/SEC)
DENSITY 1.24798E-04
(GM/CM**3)
TEMPERATURE 4709.59
(DEG K)
MASS FLOW RATE 5.76045E+03
(GM/SEC)
ENTROPY 2.3976
(CAL/GM/DEG K)
MACH NUMBER 0.3494
GAMMA 1.2754

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 32
AVERAGE STEP SIZE 0.50000E-03
CONTROLLING VARIABLE NO
RELATIVE ERROR 0.81992E-05
PREDICTOR ITERATIONS 3
ELIMINATED SPECIES NO2 N23

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
N	6.56604E-10	1.50582E-04	1.47220E-03	1	5.65986E+05	1.55295E+13
O2	8.67915E-07	1.99042E-01	-7.97902E-02	2	6.59416E+05	4.31103E+10
NO	4.23622E-09	9.71509E-04	1.90776E-02	3	-4.76294E+02	9.32585E+14
O	7.03031E-08	1.61229E-02	1.41933E-01	4	-4.00284E+06	2.82565E+14
N2	3.41507E-06	7.83192E-01	-8.84438E-03	5	-3.10432E+02	4.42517E+14
NO2	1.12757E-14	2.58591E-09	9.00713E-08	6	5.78323E+00	1.15529E+15
N2O	2.26910E-09	5.20383E-04	-1.43056E-03	7	6.46143E+05	1.1733E+12
NO*	3.93852E-15	9.03236E-10	2.68482E-08	8	-5.54290E+05	3.3345E+13
E	3.93110E-15	9.01536E-10	2.67924E-08	9	-1.72385E+00	4.48635E+15
O+	6.24788E-20	1.43285E-14	2.18262E-13	10	-1.40140E-05	1.31393E+17
O2-	5.69589E-18	1.53555E-12	4.72598E-11	11	3.59614E-03	2.84209E+17
O-	7.81999E-19	1.79339E-13	8.74855E-12	12	-5.61721E-04	6.00000E+12
MIXTURE MOLECULAR WEIGHT		28.62043	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	5.78077E+11	MASS FRACTION SUM	1.00000042

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.37006E+05	-0.33997E+02	0.23623E-07	N2	-0.15354E-02	-0.13909E-05	0.13444E-07
RHO	0.10005E-03	0.91851E-07	0.20776E-07	NO2	0.15636E-07	0.12164E-10	0.14954E-03
T	-0.44823E+04	-0.44872E+01	0.19935E-07	N2O	-0.24834E-03	-0.21211E-06	0.28141E-04
N	0.25557E-03	0.23661E-06	0.12434E-05	NO*	0.45538E-08	0.40873E-1	0.21920E-04
O2	-0.13851E-01	-0.12709E-04	0.47001E-07	E	0.45511E-08	0.40789E-1	0.21845E-04
NO	0.33118E-02	0.29633E-05	0.81992E-05	O+	0.37893E-13	0.34366E-16	0.10044E-04
O	0.24639E-01	0.22662E-04	0.74622E-06	O2-	0.82047E-11	0.71500E-1	0.29752E-04
				O-	0.15137E-11	0.12735E-14	0.32791E-03

AA
-0.73383E+00

BB
0.10636E+01

D(AREA)/D(IVAR)
0.

D2(AREA)/D(IVAR)2
0.

(1/AREA)*D(AREA)/D(IVAR)-AA
0.70383E+00

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J								
SPECIES	1	2	3	REACTION	5	6	7	8
	9	10	11	12				
N	-0.88150E-02 -0.26848E-07	0.10270E-01 -0.	0.74181E-05 0.	-0. -0.	0.96697E-05	0.	0.	-0.
O2	-0.88150E-02 -0.	0. -0.	-0. -0.56008E-10	-0.62342E-01 0.87485E-11	-0.	0.	0.	-0.86328E-02
NO	0.88150E-02 -0.	0.10270E-01 -0.	-0.74181E-05 0.	-0. -0.	-0.	-0.90071E-07	0.	-0.
O	0.88150E-02 -0.26848E-07	-0.10270E-01 -0.21826E-12	0.74181E-05 0.	0.12468E+00 -0.87485E-11	-0.	-0.90071E-07	0.10063E-01	0.86328E-02
N2	0. -0.	-0.10270E-01 -0.	-0. 0.	-0. -0.	-0.48348E-05	0.	0.10063E-01	-0.86328E-02
NO2	0. -0.	0. -0.	-0. 0.	-0. -0.	-0.	0.90071E-07	0.	-0.
N2O	0. -0.	0. -0.	-0. 0.	-0. -0.	-0.	0.	-0.10063E-01	0.86328E-02
NO+	0. 0.26848E-07	0. -0.	-0. 0.	-0. -0.	-0.	0.	0.	-0.
E	0. 0.26848E-07	0. 0.21826E-12	-0. -0.56008E-10	-0. -0.	-0.	0.	0.	-0.
O+	0. -0.	0. 0.21826E-12	-0. 0.	-0. -0.	-0.	0.	0.	-0.
O2-	0. -0.	0. -0.	-0. 0.56008E-10	-0. -0.87485E-11	-0.	0.	0.	-0.
O-	0. -0.	0. -0.	-0. 0.	-0. 0.87485E-11	-0.	0.	0.	-0.

TIME 2.20947E-06 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 1.00000E-01 CM

FLOW PROPERTIES

PRESSURE 1.69764
(ATM)
VELOCITY 43951.98
(CM/SEC)
DENSITY 1.31062E-04
(GM/CM**3)
TEMPERATURE 4433.52
(DEG K)
MASS FLOW RATE 5.76044E+03
(GM/SEC)
ENTROPY 2.4103
(CAL/GM/DEG K)
MACH NUMBER 0.3387
GAMMA 1.2834

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 6
AVERAGE STEP SIZE 0.36542E-02
CONTROLLING VARIABLE NO2
RELATIVE ERROR 0.48714E-04
PREDICTOR ITERATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
N	1.83781E-09	3.93835E-04	1.72725E-04	1	1.11502E+06	1.40238E+13
O2	7.96056E-07	1.70592E-01	-5.11863E-02	2	1.12223E+06	2.61039E+10
NO	5.56784E-08	1.40746E-02	3.83822E-02	3	-2.70912E+03	9.61182E+14
O	2.45188E-07	5.25428E-02	6.42944E-02	4	-1.76252E+06	2.99482E+14
N2	3.55704E-06	7.62259E-01	-1.89716E-02	5	-7.36317E+01	5.15343E+14
NO2	9.80586E-13	2.10136E-07	1.17571E-06	6	6.84456E+01	1.17022E+15
N2O	5.42118E-10	1.37603E-04	-3.06605E-04	7	1.20190E+05	6.91620E+11
NO+	2.05841E-13	4.41108E-08	1.69982E-07	8	-1.02340E+05	3.04206E+13
E	2.04951E-13	4.39201E-08	1.68949E-07	9	-9.89574E+00	4.91185E+15
O+	4.15480E-19	8.90356E-14	1.38804E-13	10	-8.08064E-06	1.52812E+17
O2-	3.93421E-16	8.43085E-11	3.40682E-10	11	6.01532E-02	2.99525E+17
O-	4.96956E-16	1.06496E-10	6.92589E-10	12	-4.03200E-02	6.00000E+12

MIXTURE MOLECULAR WEIGHT 28.08609 TOTAL ENERGY EXCHANGE RATE 2.71933E+11 MASS FRACTION SUM 1.00000192
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.21140E+05	-0.33775E+02	0.10294E-07	N2	-0.32934E-02	-0.52393E-05	0.31027E-08
RHO	0.63038E-04	0.10064E-06	0.75156E-08	NO2	0.20410E-06	0.30101E-09	0.48714E-04
T	-0.25186E+04	-0.40265E+01	0.15937E-07	N2O	-0.53226E-04	-0.35761E-07	0.34532E-05
N	0.29985E-04	0.49685E-07	0.13737E-05	NO+	0.29503E-07	0.46740E-10	0.63743E-05
O2	-0.88858E-02	-0.14187E-04	0.25221E-07	E	0.29329E-07	0.46460E-10	0.66871E-06
NO	0.66631E-02	0.10602E-04	0.36600E-06	O+	0.24096E-13	0.38297E-16	0.23484E-05
O	0.11161E-01	0.17858E-04	0.25236E-06	O2-	0.59142E-10	0.92641E-13	0.12234E-05
				O-	0.12223E-09	0.18765E-12	0.10702E-04

AA -0.42582E+00 BB 0.58372E+00 D(AREA)/D(IVAR) 0. D2(AREA)/D(IVAR)2 0. (1/AREA)*D(ARC)/D(IVAR)-AA 0.42582E+00

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J								
SPECIES	1	2	3	REACTION	5	6	7	8
	9	10	11	12				
N	-0.19153E-01 -0.16998E-06	0.19277E-01 -0.	0.46535E-04 0.	-0. -0.	0.25296E-05	0.	0.	-0.
O2	-0.19153E-01 -0.	0. -0.	-0. -0.10333E-08	-0.30275E-01 0.69259E-09	-0.	0.	0.	-0.17579E-02
NO	0.19153E-01 -0.	0.19277E-01 -0.	-0.46535E-04 0.	-0. -0.	-0.	-0.11757E-05	0.	-0.
O	0.19153E-01 -0.16998E-06	-0.19277E-01 -0.13880E-12	0.46535E-04 0.	-0.60551E-01 -0.69259E-09	-0.	-0.11757E-05	0.20645E-02	0.17579E-02
N2	0. -0.	-0.19277E-01 -0.	-0. 0.	-0. -0.	-0.12648E-05	0.	0.20645E-02	-0.17579E-02
NO2	0. -0.	0. -0.	-0. 0.	-0. -0.	-0.	0.11757E-05	0.	-0.
N2O	0. -0.	0. -0.	-0. 0.	-0. -0.	-0.	0.	-0.20645E-02	0.17579E-02
NO+	0. 0.16998E-06	0. -0.	-0. 0.	-0. -0.	-0.	0.	0.	-0.
E	0. 0.16998E-06	0. 0.13880E-12	-0. -0.10333E-08	-0. -0.	-0.	0.	0.	-0.
O+	0. -0.	0. 0.13880E-12	-0. 0.	-0. -0.	-0.	0.	0.	-0.
O2-	0. -0.	0. -0.	-0. 0.10333E-08	-0. -0.69259E-09	-0.	0.	0.	-0.
O-	0. -0.	0. -0.	-0. 0.	-0. 0.69259E-09	-0.	0.	0.	-0.

TIME 6.92847E-06 SEC

AREA 1.00000E+03 SQ CM

AXIAL POSITION 3.00000E-01 CM

FLOW PROPERTIES

PRESSURE 1.71308
(ATM)
VELOCITY 41235.29
(CM/SEC)
DENSITY 1.39697E-04
(GM/CM**3)
TEMPERATURE 4121.39
(DEG K)
MASS FLOW RATE 5.76044E+03
(GM/SEC)
ENTROPY 2.4195
(CAL/GM/DEG K)
MACH NUMBER 0.3254
GAMMA 1.2923

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 31
AVERAGE STEP SIZE 0.65029E-02
CONTROLLING VARIABLE V
RELATIVE ERROR 0.58628E-06
PREDICTOR ITERATIONS 3
ELIMINATED SPECIES NO2 N2O

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
N	1.90403E-09	3.75880E-04	-5.82216E-05	1	5.49103E+05	1.23545E+13
O2	6.84081E-07	1.35047E-01	-2.20719E-02	2	5.43743E+05	1.36525E+10
NO	2.16488E-07	4.27375E-02	2.12780E-02	3	-2.36386E+03	9.96915E+14
O	4.44187E-07	8.76882E-02	2.28894E-02	4	-5.64632E+05	3.21223E+14
N2	3.71867E-06	7.34114E-01	-1.05817E-02	5	-1.09048E+01	5.44347E+14
NO2	1.04639E-11	2.06572E-06	3.01664E-06	6	1.54579E+02	1.18980E+15
N2O	1.78349E-10	3.52084E-05	-2.97355E-05	7	1.87997E+04	4.20082E+11
NO+	1.13098E-12	2.23270E-07	1.76151E-07	8	-1.72760E+04	2.44817E+13
E	1.11974E-12	2.21052E-07	1.73210E-07	9	-9.02633E+00	5.48028E+15
O+	7.67254E-19	1.51466E-13	3.08235E-14	10	-1.57946E-06	1.33409E+17
O2-	2.27948E-15	4.49998E-10	3.58196E-10	11	1.50722E-01	3.18931E+17
O-	8.95872E-15	1.76857E-09	2.58318E-09	12	-1.32367E-01	6.00000E+12

MIXTURE MOLECULAR WEIGHT 27.57797

TOTAL ENERGY EXCHANGE RATE
(CAL-CM**3/GM**2/SEC)

9.30207E+10

MASS FRACTION SUM

1.00000399

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.87573E+04	-0.53159E+02	0.23952E-07	N2	-0.18370E-02	-0.11153E-04	0.37689E-08
RHO	0.29668E-04	0.17986E-06	0.17687E-07	NO2	0.52353E-06	0.26779E-08	0.15835E-04
T	-0.98100E+03	-0.59565E+01	0.30016E-07	N2O	-0.51623E-05	-0.32783E-07	0.44694E-05
N	-0.10107E-04	-0.59561E-07	0.58628E-06	NO+	0.30579E-07	0.18434E-09	0.94339E-07
O2	-0.38316E-02	-0.23264E-04	0.83396E-07	E	0.30069E-07	0.18131E-09	0.13203E-06
NO	0.36938E-02	0.22428E-04	0.12651E-06	O+	0.53509E-14	0.32380E-16	0.76792E-05
O	0.39735E-02	0.24127E-04	0.19267E-06	O2-	0.52192E-10	0.37936E-12	0.90923E-05
				O-	0.44843E-09	0.26458E-11	0.48246E-05

AA
-0.13988E+00

BB
0.24460E+00

D(AREA)/D(IVAR)
0.

D2(AREA)/D(IVAR)2
0.

(1/AREA)*D(AREA)/D(IVAR)-AA
0.129.8E+00

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J								
SPECIES	1 9	2 10	3 11	REACTION 4 12	5	6	7	8
N	-0.10716E-01 -0.17615E-06	0.10611E-01 -0.	0.46131E-04 0.	-0. -0.	0.42562E-06	0.	0.	-0.
O2	-0.10716E-01 -0.	0. -0.	-0. -0.29414E-08	-0.11019E-01 0.25832E-08	-0.	0.	0.	-0.33714E-03
NO	0.10716E-01 -0.	0.10611E-01 -0.	-0.46131E-04 0.	-0. -0.	-0.	-0.30166E-05	0.	-0.
O	0.10716E-01 -0.17615E-06	-0.10611E-01 -0.30824E-13	0.46131E-04 0.	0.22038E-01 -0.25832E-08	-0.	-0.30166E-05	0.36688E-03	0.33714E-03
N2	0. -0.	-0.10611E-01 -0.	-0. 0.	-0. -0.	-0.21281E-06	0.	0.36688E-03	-0.33714E-03
NO2	0. -0.	0. -0.	-0. 0.	-0. -0.	-0.	0.30166E-05	0.	-0.
N2O	0. -0.	0. -0.	-0. 0.	-0. -0.	-0.	0.	-0.36688E-03	0.33714E-03
NO+	0. 0.17615E-06	0. -0.	-0. 0.	-0. -0.	-0.	0.	0.	-0.
E	0. 0.17615E-06	0. 0.30824E-13	-0. -0.29414E-08	-0. -0.	-0.	0.	0.	-0.
O+	0. -0.	0. 0.30824E-13	-0. 0.	-0. -0.	-0.	0.	0.	-0.
O2-	0. -0.	0. -0.	-0. 0.29414E-08	-0. -0.25832E-08	-0.	0.	0.	-0.
O-	0. -0.	0. -0.	-0. 0.	-0. 0.25832E-08	-0.	0.	0.	-0.

TIME 2.45511E-05 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 1.00000E+00 CM

FLOW PROPERTIES

PRESSURE 1.72854
(ATM)
VELOCITY 38516.28
(CM/SEC)
DENSITY 1.49559E-04
(GM/CM**3)
TEMPERATURE 3815.59
(DEG K)
MASS FLOW RATE 5.76044E+03
(GM/SEC)
ENTROPY 2.4236
(CAL/GM/DEG K)
MACH NUMBER 0.3120
GAMMA 1.3013

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 40
AVERAGE STEP SIZE 0.17650E-01
CONTROLLING VARIABLE N2O
RELATIVE ERROR 0.92532E-05
PREDICTOR ITERATIONS 11

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
N	1.54073E-09	2.79074E-04	-1.05584E-05	1	2.82154E+04	1.07593E+13
O2	5.65279E-07	1.02390E-01	-3.37922E-03	2	2.69871E+04	6.52789E+09
NO	3.70134E-07	6.70427E-02	1.21577E-03	3	-7.56753E+02	1.03609E+15
O	5.71424E-07	1.21616E-01	5.53999E-03	4	-1.20796E+05	3.45814E+14
N2	3.91237E-06	7.08653E-01	-6.02164E-04	5	-1.01424E+00	5.76749E+14
NO2	5.24306E-11	9.49682E-06	2.05999E-06	6	9.20964E+01	1.21248E+15
N2O	4.89868E-11	8.87304E-06	-1.50019E-06	7	2.13135E+03	2.38145E+11
NO+	3.18774E-12	5.77400E-07	5.79153E-08	8	-2.06428E+03	1.86216E+13
E	3.11843E-12	5.64846E-07	5.52351E-08	9	-2.58923E+00	6.15212E+15
O+	7.99607E-19	1.41060E-13	3.29124E-15	10	-1.47142E-07	2.22395E+17
O2-	6.55472E-15	1.18726E-09	8.70285E-11	11	1.19827E-01	3.40503E+17
O-	5.27563E-14	1.13671E-08	2.59322E-09	12	-1.15936E-01	6.00000E+12

MIXTURE MOLECULAR WEIGHT 27.08972 TOTAL ENERGY EXCHANGE RATE 1.58710E+10 (CAL-CM**3/GM**2/SEC) MASS FRACTION SUM 1.00000587

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.16834E+04	-0.41002E+02	0.26820E-05	V2	-3.10453E-03	-0.26861E-05	0.11856E-06
RHO	0.65367E-05	0.15904E-06	0.23639E-06	NO2	0.35761E-06	0.58117E-08	0.38041E-05
T	-0.19525E+03	-0.47502E+01	0.29077E-06	N2O	-0.25043E-06	-0.71065E-08	0.92532E-05
N	-0.18329E-05	-0.43077E-07	0.18551E-05	NO+	0.10354E-07	0.24483E-07	0.15902E-05
O2	-0.58663E-03	-0.14364E-04	0.13262E-05	E	0.95887E-08	0.23369E-09	0.15990E-05
NO	0.21106E-03	0.54225E-05	0.25160E-05	O+	0.57135E-15	0.13882E-17	0.74860E-06
O	0.96173E-03	0.23298E-04	0.84620E-06	O2-	0.15108E-10	0.53031E-12	0.13809E-05
				O-	0.45318E-09	0.10609E-10	0.12865E-05

AA -0.39452E-01 BB 0.52452E-01 D(AREA)/D(IVAR) 0. D2(AREA)/D(IVAR)2 0. (1/AREA)*D(AREA)/D(IVAR)-AA 0.39452E-01

OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J								
SPECIES	1	2	3	REACTION	5	6	7	8
	9	10	11	12				
N	-0.63111E-03 -0.57915E-07	0.0364E-03 -0.	0.16927E-04 0.	-0. -0.	0.45372E-07	0.	0.	-0.
O2	-0.63111E-03 -0.	0. -0.	-0. -0.26803E-08	-0.27019E-02 0.25932E-08	-0.	0.	0.	-0.46173E-04
NO	0.63111E-03 -0.	0.0364E-03 -0.	-0.16927E-04 0.	-0. -0.	-0.	-0.20600E-05	0.	-0.
O	0.63111E-03 -0.57915E-07	-0.60364E-03 -0.32912E-14	0.16927E-04 0.	0.54039E-02 -0.25932E-08	-0.	-0.20600E-05	0.47674E-04	0.46173E-04
N2	0. -0.	-0.60364E-03 -0.	-0. 0.	-0. -0.	-0.22686E-07	0.	0.47674E-04	-0.46173E-04
NO2	0. -0.	0. -0.	-0. 0.	-0. -0.	-0.	0.20600E-05	0.	-0.
N2O	0. -0.	0. -0.	-0. 0.	-0. -0.	-0.	0.	-0.47674E-04	0.46173E-04
NO+	0. 0.57915E-07	0. -0.	-0. 0.	-0. -0.	-0.	0.	0.	-0.
E	0. 0.57915E-07	0. 0.32912E-14	-0. -0.26803E-08	-0. -0.	-0.	0.	0.	-0.
O+	0. -0.	0. 0.32912E-14	-0. 0.	-0. -0.	-0.	0.	0.	-0.
O2-	0. -0.	0. -0.	-0. 0.26803E-08	-0. -0.25932E-08	-0.	0.	0.	-0.
O-	0. -0.	0. -0.	-0. 0.	-0. 0.25932E-08	-0.	0.	0.	-0.

TIME 2.65890E-04 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 1.00000E+01 CM

FLOW PROPERTIES

PRESSURE 1.73751
(ATM)
VELOCITY 36937.72
(CM/SEC)
DENSITY 1.55950E-04
(GM/CM**3)
TEMPERATURE 3622.45
(DEG K)
MASS FLOW RATE 5.76043E+03
(GM/SEC)
ENTRJPY 2.4243
(CAL/GM/DEG K)
MACH NUMBER 0.3040
GAMMA 1.3082

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 57
AVERAGE STEP SIZE 0.10575E+00
CONTROLLING VARIABLE NO2
RELATIVE ERROR 0.28647E-06
PREDICTOR ITERATIONS 11

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOL FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	RATE CONSTANT (CGS UNITS)
N	1.43368E-09	2.45267E-04	-9.45584E-09	1	-1.11924E+02	9.77550E+12
O2	5.27368E-07	9.02195E-02	-2.07474E-06	2	-1.13369E+02	3.84156E+09
NO	3.32611E-07	5.69014E-02	-5.50931E-06	3	-1.05111E+00	1.06336E+15
O	9.77529E-07	1.50123E-01	9.65077E-06	4	-1.95026E+02	3.63382E+14
N2	4.10632E-06	7.02489E-01	2.75815E-06	5	-9.09406E-04	5.99661E+14
NO2	9.92664E-11	1.69820E-05	4.55121E-09	6	1.87136E-01	1.22905E+15
N2O	2.17939E-11	3.72839E-06	-9.99862E-10	7	2.24826E+00	1.58385E+11
NO+	3.79428E-12	6.49102E-07	-7.55910E-11	8	-2.20715E+00	1.54339E+13
E	3.65218E-12	6.24796E-07	-7.67784E-11	9	3.10814E-03	6.65065E+15
O+	1.20945E-18	2.06906E-13	4.38453E-16	10	-1.80283E-08	2.53235E+17
O2-	8.33806E-15	1.42643E-09	6.52877E-15	11	4.88415E-05	3.55669E+17
O-	1.33738E-13	2.28792E-08	1.18131E-12	12	-4.85731E-05	6.00000E+12

MIXTURE MOLECULAR WEIGHT 26.67907 TOTAL ENERGY EXCHANGE RATE 1.87019E+07 MASS FRACTION SUM 1.00000596
(CAL-CM**3/GM**2/SEC)

VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR	VARIABLE	DERIVATIVE	INCREMENT	RELATIVE ERROR
V	-0.20213E+01	-0.32425E+00	0.73288E-08	N2	0.47881E-06	0.74824E-07	0.27250E-08
RHD	0.85337E-08	0.13690E-08	0.75229E-08	NO2	0.79008E-09	0.59140E-10	0.28647E-06
T	-0.25511E+00	-0.40837E-01	0.97665E-08	N2O	-0.17357E-09	-0.24406E-10	0.11152E-06
N	-0.16415E-08	-0.17194E-09	0.56237E-07	NO+	-0.13122E-10	-0.20537E-11	0.78019E-07
O2	-0.36017E-06	-0.58692E-07	0.13853E-07	E	-0.13329E-10	-0.20826E-11	0.84012E-07
NO	-0.95641E-06	-0.14948E-06	0.67111E-07	O+	0.75115E-16	0.11294E-16	0.
O	0.16754E-05	0.26678E-06	0.42025E-07	O2-	0.11334E-14	-0.34910E-14	0.18233E-06
				O-	0.20507E-12	0.32388E-13	0.92158E-07

AA 0.49665E-04 HB 0.71983E-04 D(AREA)/D(IVAR) 0. D2(AREA)/D(IVAR)2 0. (1/AREA)*D(ARL)/D(IVAR)-AA 0.45661E-04

SPECIES	OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J							
	1 9	2 10	3 11	REACTION 4 12	5	6	7	8
N	0.27220E-05 0.75591E-10	-0.27572E-05 -0.	0.25563E-07 0.	-0. -0.	0.44234E-10	0.	0.	-0.
O2	0.27220E-05 0.	-0. -0.	-0. -0.11878E-11	-0.47431E-05 0.11813E-11	-0.	0.	0.	-0.53679E-07
NO	-0.27220E-05 0.	-0.27572E-05 -0.	-0.25563E-07 0.	-0. -0.	-0.	-0.45512E-08	0.	-0.
O	-0.27220E-05 0.75591E-10	0.27572E-05 -0.43845E-15	0.25563E-07 0.	0.94862E-05 -0.11813E-11	-0.	-0.45512E-08	0.54678E-07	0.53679E-07
N2	-0. 0.	0.27572E-05 -0.	-0. 0.	-0. -0.	-0.22117E-10	0.	0.54678E-07	-0.53679E-07
NO2	-0. 0.	-0. -0.	-0. 0.	-0. -0.	-0.	0.45512E-08	0.	-0.
N2O	-0. 0.	-0. -0.	-0. 0.	-0. -0.	-0.	0.	-0.54678E-07	0.53679E-07
NO+	-0. -0.75591E-10	-0. -0.	-0. 0.	-0. -0.	-0.	0.	0.	-0.
E	-0. -0.75591E-10	-0. 0.43845E-15	-0. -0.11878E-11	-0. -0.	-0.	0.	0.	-0.
O+	-0. 0.	-0. 0.43845E-15	-0. 0.	-0. -0.	-0.	0.	0.	-0.
O2-	-0. 0.	-0. -0.	-0. 0.11878E-11	-0. -0.11813E-11	-0.	0.	0.	-0.
O-	-0. 0.	-0. -0.	-0. 0.	-0. 0.11813E-11	-0.	0.	0.	-0.

(GCKP) END OF THIS CASE - READ DATA FOR NEXT CASE

APPENDIX F

AVAILABILITY OF THERMODYNAMIC AND RATE CONSTANT DATA

Thermodynamic Data

The form of the thermodynamic data equations has already been discussed under the heading Thermodynamic Data and Species Names in the section GENERAL DESCRIPTION OF PROGRAM USE. Curve fitted coefficients A_1, A_2, \dots, A_7 have been calculated for 415 species by Gordon and McBride. The complete list of coefficients has been published in reference 13. Two sets of coefficients are given for each species. The first listed set was obtained for the temperature range 1000 to 5000 K. The second set was curve fitted for the temperature range 300 to 1000 K. The high-range equation can be extrapolated beyond the high temperature limit to 6000 K and the low range equation can be used down to 100 K. These coefficients will be available as part of the chemical kinetics program.

Rate Constant Data

No set of "standard" reaction rate constants can be given analogous to the sets of coefficients for thermodynamic properties of the species. Rate constant data are much less precisely known. In general, the choice of rate constant for any reaction is left to the user. For the convenience of the reader a short list of rate constant equations is presented in table V. These rate constants are not to be taken necessarily as "best" values but only as reasonable values to use in performing kinetics calculations. Additional rate constant data are found in the sample case data listed in appendix E. Further kinetics information may be found in references 22 to 28 and 30.

TABLE V. - REACTION RATE CONSTANTS^a

$$[k_j = A_j T^{n_j} \exp(-E_j/RT).]$$

Reaction number	Reaction	A _j	n _j	E _j , cal/mole	Reference
1	H + O ₂ → OH + O	1.25×10 ¹⁴	0	16 300	29
2	O + H ₂ → OH + H	2.96×10 ¹³	↓	9 800	29
3	H ₂ + OH → H ₂ O + H	2.1×10 ¹³	↓	5 100	29
4	O + H ₂ O → OH + OH	5.75×10 ¹³	↓	18 000	22
5	H ₂ + HO ₂ → H ₂ O ₂ + H	9.6×10 ¹²	↓	24 000	23
6	H + HO ₂ → OH + OH	7.0×10 ¹³	↓	0	30
7	OH + HO ₂ → H ₂ O + O ₂	6.0×10 ¹²	↓	0	30
8	O + HO ₂ → OH + O ₂	6.0×10 ¹²	↓	0	30
9	HO ₂ + HO ₂ → H ₂ O ₂ + O ₂	1.8×10 ¹²	↓	0	30
10	H + H ₂ O ₂ → H ₂ O + OH	3.18×10 ¹⁴	↓	9 000	23
11	OH + H ₂ O ₂ → H ₂ O + HO ₂	1.0×10 ¹³	↓	1 800	23
12	H + O ₂ + Ar → HO ₂ + Ar	1.59×10 ¹⁵	↓	-1 000	23
13	H ₂ O ₂ + N ₂ → OH + OH + N ₂	1.17×10 ¹⁷	↓	45 500	23
14	H + HO ₂ → H ₂ + O ₂	2.3×10 ¹³	↓	0	28
15	H + H + Ar → H ₂ + Ar	1.0×10 ¹⁸	-1.0	0	31
16	O ₂ + Ar → O + O + Ar	2.55×10 ¹⁸	-1.0	118 700	32
17	H + OH + Ar → H ₂ O + Ar	7.5×10 ²³	-2.6	0	33
18	CO + OH → CO ₂ + H	4.2×10 ¹¹	0	1 000	29
19	CO + O ₂ → CO ₂ + O	1.6×10 ¹³	0	41 000	29
20	H ₂ + O ₂ → OH + OH	1.0×10 ¹³	0	43 000	(b)
21	N + O + N ₂ → NO + N ₂	6.4×10 ¹⁶	-0.5	0	24
22	N + O ₂ → NO + O	6.4×10 ⁹	1.0	6 250	24
23	O + N ₂ → NO + N	1.36×10 ¹⁴	0	75 400	24
24	NO ₂ + O → NO + O ₂	1.0×10 ¹³	↓	600	25
25	NO + O + Ar → NO ₂ + Ar	1.05×10 ¹⁵	↓	-1 870	25
26	NO ₂ + H → NO + OH	7.2×10 ¹⁴	↓	1 930	30
27	NO + HO ₂ → NO ₂ + OH	1.0×10 ¹³	↓	0	28

^aUnits of bimolecular and two-body dissociation reaction rate constants are cm³ mole⁻¹ sec⁻¹. Units of three-body recombination reaction rate constants are cm⁶ mole⁻² sec⁻¹.

^bAuthors' estimate.

APPENDIX G

FORTRAN PROGRAM LISTING AND FLOW CHARTS

\$IBFTC GCKP	DECK	AA001
C	GENERAL CHEMICAL KINETICS PROGRAM	AA002
	LOGICAL NEXT, EVSTEP	AA003
	REAL IVAR	AA004
	COMMON/COND/DUM1(4), IVAR, Y(28), DUM2(2), NEXT	AA005
	COMMON/SINT/HMIN, HINT, HN, HNP1, HMAX, NH, AVH, EMAX, ERP, JCV, KOUNT, ERFP	AA006
	COMMON/PQRE/PK(28), QK(28), RK(28), E(28)	AA007
	COMMON/PRIN/PRINT(50), NPRNTS, END, EVSTEP	AA008
C	READ AND CONVERT INPUT, PERFORM PRE-KINETIC CALCULATIONS	AA009
	CALL KINF	AA010
	1 IF (NEXT) GO TO 1000	AA011
C	PRINT REACTIONS, ASSIGNED VARIABLE PROFILE, INTEGRATION CONTROLS	AA012
	CALL OUT1	AA013
C	COMPUTE (NON-INPUT) INITIAL CONDITIONS	AA014
	CALL PRED1	AA015
C	PRINT ALL INITIAL CONDITIONS	AA016
	CALL OUT2	AA017
	IF (NEXT) GO TO 1000	AA018
C	INITIAL INTEGRATION STEPS	AA019
	CALL INTI	AA020
	NH = 2	AA021
	AVH = HINT	AA022
	CALL OUT3	AA023
	IF (NEXT) GO TO 1000	AA024
	IF (.NOT. EVSTEP) GO TO 3	AA025
C	** INTEGRATION - PRINT RESULTS AFTER EVERY STEP	AA026
	2 NH = 0	AA027
	PREV = IVAR	AA028
	CALL INTG	AA029
	NH = NH + 1	AA030
	AVH = HN	AA031
	IF (NH .NE. 1) AVH = (IVAR - PREV)/FLOAT(NH)	AA032
	CALL OUT3	AA033
	IF (NEXT) GO TO 1000	AA034
	HTOP = END - IVAR	AA035
	IF (HTOP .LE. 0.) GO TO 100	AA036
	IF ((HTOP-HNP1) .LT. 0.) HNP1 = HTOP	AA037
	GO TO 2	AA038
C	LOCATE FIRST PRINT STATION	AA039
	3 DO 4 I=1, NPRNTS	AA040
	IF (PRINT(I) .GT. IVAR) GO TO 5	AA041
	4 CONTINUE	AA042
		AA043
		AA044
		AA045
		AA046
		AA047
		AA048
		AA049
		AA050
		AA051
		AA052
		AA053

5 NS = I	AA054
C ** INTEGRATION - PRINT RESULTS AT PRINT STATIONS	AA055
DO 10 I=NS,NPRNTS	AA056
NH = 0	AA057
PREV = IVAR	AA058
	AA059
C SET NEXT PRINT STATION	AA060
PRNT = PRINT(I)	AA061
C INTEGRATE TO PRINT STATION	AA062
6 HTOP = PRNT - IVAR	AA063
IF (HTOP .LE. HNP1) GO TO 7	AA064
CALL INTG	AA065
NH = NH + 1	AA066
IF (NEXT) GO TO 8	AA067
GO TO 6	AA068
	AA069
C SPECIAL STEP TO PRINT STATION	AA070
7 CALL CASG (HN,OK,HTOP,RK)	AA071
ERRN = ERROR(Y,RK,E,JCV,HTOP)	AA072
CALL PRED	AA073
NH = NH + 1	AA074
8 AVH = (IVAR - PREV)/FLOAT(NH)	AA075
CALL OUT3	AA076
IF (NEXT) GO TO 1000	AA077
CALL INTC	AA078
	AA079
	AA080
10 CONTINUE	AA081
	AA082
100 WRITE (6,101)	AA083
101 FORMAT (7H0(GCKP),5X,44HEND OF THIS CASE - READ DATA FOR NEXT CA	AA084
*SE)	AA085
CALL RINP	AA086
GO TO 1	AA087
	AA088
1000 WRITE (6,1001)	AA089
1001 FORMAT (7H0(GCKP),5X,46HA FATAL ERROR HAS OCCURRED - CASE TERMIN	AA090
*ATED)	AA091
CALL RINP	AA092
GO TO 1	AA093
	AA094
END	AA095
\$IEFTC KINPP DECK	
SUBROUTINE KINP	AB001
	AB002
C INPUT CAN BE ACCEPTED IN (1) INTERNAL (CGS) UNITS, (2) FPS UNITS,	AB003
C (3) SI UNITS	AB004
	AB005
C THE FOLLOWING UNITS ARE USED INTERNALLY	AB006
C * DISTANCE CM *	AB007
C * AREA CM**2 *	AB008
C * MASS FLOW RATE GM/SEC *	AB009
C * PRESSURE ATM *	AB010
C * TIME SEC *	AB011
C * VELOCITY CM/SEC *	AB012
C * DENSITY GM/CC *	AB013
C * TEMPERATURE DEG K *	AB014
C * CONCENTRATION MOLE(I)/MASS *	AB015
	AB016
C INTERNAL CORRESPONDENCE	AB017
C * DVAR - DEPENDENT VARIABLE *	AB018
C * IVAR - INDEPENDENT VARIABLE *	AB019

C	* AVAR - ASSIGNED VARIABLE *	AB020
		AB021
C	THE FOLLOWING LOGICAL TAPE UNITS ARE REQUIRED	AB022
C	* LTHM (4) - FOR THERMODYNAMIC DATA *	AB023
C	* LDAT (7) - FOR TEMPORARY STORAGE OF DATA CARDS *	AB024
C	LOGICAL TAPE UNIT ASSIGNMENTS ARE SPECIFIED IN 'NAMBLK'	AB025
		AB026
	DOUBLE PRECISION DSP,DSPP,DSPNM,DALSP	AB027
		AB028
	LOGICAL ALLM1,CONC,DBUGO,ELIM,EVSTEP,EXCHR,MOLEF,MMHG	AB029
	LOGICAL COMBUS,RHOCON,SHOCK,TCON	AB030
	LOGICAL NEWPRT,NEXT	AB031
		AB032
	REAL MDOT,IVAR,M,MW,N,LSUBM,MIXMW,M2,NEW	AB033
		AB034
	DIMENSION ISS(25),TBR(3),CXTB(40),CATB(40),APPINT(50),THMC(7,2)	AB035
	DIMENSION SP(2,4),DSP(4),SPP(2,3),DSPP(3),SPNM(2,27),DSPNM(27)	AB036
	DIMENSION SPT(2),LMT(4),SUBS(4),C(25),CX(4)	AB037
	DIMENSION CUA(2),FUA(2),SUA(2),CUP1(2),CUP2(2),FUP(2),SUP(2)	AB038
		AB039
	COMMON/LTUS/LTHM,LDAT	AB040
	COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,ELIM,TCON,RHOCON,IPPCOD	AB041
	COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT	AB042
	COMMON/REAC/LSR(4,30),XX(30),RATE(30),LKEQ(30),DLKEQ(30),MM(30),LB	AB043
	COMMON/RRAT/A(30),N(30),EACT(30),B(30),M(25,30),ALLM1	AB044
	COMMON/AFUN/CN(4),ITPSZ,LSUBM,ETA,D,VISC,BETA	AB045
	COMMON/SPEC/SNAM(2,30),MW(25),W(25),STOIC(25,30),OMEGA(25,30)	AB046
	COMMON/SINT/HMIN,HI,HN,HNP1,HMAX,NH,AVH,EMAX,ERRN,JCV,KOUNT,ERRP	AB047
	COMMON/TCOF/TC(7,2,25),TLOW,TMID,THI	AB048
	COMMON/PRIN/PRINT(50),NP,CEND,EVSTEP	AB049
	COMMON/XVSA/XTB(40),ATB(40),NT,XU,AU(2),CX3,CX2,CX1,CX0	AB050
	COMMON/SNMW/DALSP(75),ALMW(75)	AB051
	COMMON/KOUT/TITLE(20),UNITI,UNITO,CONC,EXCHR,DELH(30),FPS,SI,DBUGO	AB052
	COMMON/GHSC/GBT(25),HRT(25),SR(25),CPR(25),DCPR(25)	AB053
	COMMON/PQRE/PK(28),QK(28),RK(28),E(28)	AB054
	COMMON/SKIP/NEGL(25),I1,I2,IT	AB055
	COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R	AB056
	COMMON/MISC/TT,PP,CPR0,HRO,ENN,SUMN,ENNL,LLMT(15),B0(15)	AB057
	COMMON/INDX/TP,HP,NLM,NS,IQ1,CONVG,KMAT,IMAT	AB058
		AB059
	EQUIVALENCE (C,SIGMA),(SPNM,DSPNM),(SP,DSP),(SPP,DSPP),(SPT,SP)	AB060
	EQUIVALENCE (SPNM,SNAM(1,4)),(EFFM,SPNM(1,26)),(BLANK,SPNM(1,27))	AB061
	EQUIVALENCE (CX3,CX)	AB062
		AB063
	DATA CU,FU,SU/2HCM,2HFT,2HM /	AB064
	DATA CUA/4HCM**,1H2/,FUA/4HFT**,1H2/,SUA/4HM**2,1H /	AB065
	DATA CUP1/4HMMHG,1H /,CUP2/3HATM,1H /,FUP/4HLB/F,4HT**2/,SUP/4HN/M	AB066
	**2H*2/	AB067
	DATA NEW,CHANGE,REPEAT/3HNEW,4HCHAN,4HREPE/	AB068
	DATA TAPEND,CARDS/3HEND,4HCARD/	AB069
		AB070
	NAMLIST/PROB/HMIN,HMAX,HINT,EMAX,ALLM1,ELIM,CONC,EXCHR,	AB071
	* IPRCOD,ITPSZ,XTB,ATB,NTB,CX3,CX2,CX1,CX0,LSUBM,ETA,D,VISC,BETA	AB072
	*,END,DELP,PRINT,NPRNTS,APRINT,EVSTEP,DBUGO,	AB073
	* COMBUS,SHOCK,TCON,RHOCON	AB074
		AB075
		AB076
C	THERMODYNAMIC DATA WILL BE INPUT FROM 'UNIT'	AB077
	READ (5,99) UNIT	

99	FORMAT (20A4)	AB078
	IF (UNIT .NE. CARDS) GO TO 3	AB079
	REWIND LTHM	AB080
	READ (5,98) TLOW,TMID,THI	AB081
98	FORMAT (3F10.3)	AB082
	WRITE (LTHM,98) TLOW,TMID,THI	AB083
1	READ (5,97) (SPT(I),I=1,2), (LMT(I),SUBS(I),I=1,4)	AB084
97	FORMAT (2A4,16X,4(A2,F3.0))	AB085
C	'END' CARD SIGNALS END OF THERMODYNAMIC DATA	AB086
	IF (SPT(1) .EQ. TAPEND) GO TO 2	AB087
	WRITE (LTHM,97) (SPT(I),I=1,2), (LMT(I),SUBS(I),I=1,4)	AB088
	READ (5,96) ((THMC(K,I),K=1,7),I=1,2)	AB089
96	FORMAT (5E15.8)	AB090
	WRITE (LTHM,96) ((THMC(K,I),K=1,7),I=1,2)	AB091
	GO TO 1	AB092
2	WRITE (LTHM,99) TAPEND	AB093
	REWIND LTHM	AB094
		AB095
		AB096
3	CALL CIMAGE	AB097
C	READ OUTPUT TITLE	AB098
	READ (LDAT,99) TITLE	AB099
	ACTION = NEW	AB100
	GO TO 4	AB101
		AB102
	ENTRY RINP	AB103
	NEXT = .FALSE.	AB104
	CALL CIMAGE	AB105
C	READ NEW OUTPUT TITLE	AB106
	READ (LDAT,99) TITLE	AB107
C	READ ACTION SWITCH	AB108
	READ (LDAT,99) ACTION	AB109
		AB110
	IF (ACTION .NE. NEW) GO TO 9	AB111
C	SET STANDARD OPTIONS	AB112
4	CONC = .TRUE.	AB113
	EXCHR = .FALSE.	AB114
	COMBUS = .FALSE.	AB115
	SHOCK = .FALSE.	AB116
	TCON = .FALSE.	AB117
	RHOCON = .FALSE.	AB118
	ELIM = .TRUE.	AB119
	EVSTEP = .FALSE.	AB120
	DEBUGO = .FALSE.	AB121
	EMAX = 0.0001	AB122
	ITPSZ = 5	AB123
	ALLM1 = .TRUE.	AB124
	DO 5 I=1,25	AB125
	DO 5 J=1,30	AB126
5	M(I,J) = 1.	AB127
		AB128
C	INITIALIZE	AB129
	NEXT = .FALSE.	AB130
	HINT = 0.	AB131
	NLM = 0	AB132
	NS = 0	AB133
	LS = 0	AB134
	LR = 0	AB135
	NT = 0	AB136
	DO 6 I=1,40	AB137
	XTR(I) = 0.	AB138
	CXTR(I) = 0.	AB139
	ATB(I) = 0.	AB140

6 CATB(I) = 0.	AB141
UNCEND = 0.	AB142
CEND = 0.	AB143
NP = 0	AB144
DO 7 I=1,50	AB145
7 PRINT(I) = 0.	AB146
DO 8 I=1,25	AB147
DO 8 J=1,30	AB148
8 STOIC(I,J) = 0.	AB149
LSUBM = 0.	AB150
ETA = 0.	AB151
D = 0.	AB152
VISC = 0.	AB153
BETA = 0.	AB154
CX3 = 0.	AB155
CX2 = 0.	AB156
CX1 = 0.	AB157
CX0 = 0.	AB158
GO TO 14	AB159
9 IF (ACTION .NE. CHANGE) GO TO 13	AB160
C READ REACTION AND (CHANGED) REACTION RATE	AB161
10 READ (LDAT,95) ((SP(K,I),K=1,2),I=1,4),TA,TN,TEA	AB162
95 FORMAT (2(2A4,1X),1X,2(1X,2A4),4X,F15.5,2(2X,F10.5))	AB163
C BLANK CARD SIGNALS END OF CHANGE REACTION LIST	AB164
IF (SP(1,2) .EQ. BLANK) GO TO 12	AB165
C SEARCH INPUT REACTION LIST	AB166
DO 11 J=1,LR	AB167
N1 = LSR(1,J)	AB168
N2 = LSR(2,J)	AB169
N3 = LSR(3,J)	AB170
IF (N1 .EQ. 0) N1 = 26	AB171
IF (N1 .LT. 0) N1 = 27	AB172
IF (DSPNM(N1) .NE. DSP(1) .OR. DSPNM(N2) .NE. DSP(2) .OR. DSPNM(N3	AB173
*) .NE. DSP(3)) GO TO 11	AB174
A(J) = TA	AB175
N(J) = TN	AB176
EACT(J) = TEA	AB177
GO TO 10	AB178
11 CONTINUE	AB179
C ERROR MESSAGE - NO MATCH FOUND	AB180
WRITE (6,101) ((SP(K,I),K=1,2),I=1,4)	AB181
101 FORMAT (7H0(KINP),5X,55HTHE INPUT REACTION LIST DOES NOT CONTAIN T	AB182
*HE REACTION ,2A4,3H + ,2A4,3H = ,2A4,3H + ,2A4)	AB183
NEXT = .TRUE.	AB184
GO TO 10	AB185
12 READ (LDAT,99) ACTION	AB186
13 IF (ACTION .EQ. REPEAT) GO TO 33	AB187
14 LSOLD = LS	AB188
LROLD = LR	AB189
C READ (NEW OR ADDED) REACTION AND REACTION RATE	AB190
15 READ (LDAT,95) ((SP(K,I),K=1,2),I=1,4),TA,TN,TEA	AB191
C BLANK CARD SIGNALS END OF NEW OR ADD REACTION LIST	AB192
IF (SP(1,2) .EQ. BLANK) GO TO 21	AB193
LR = LR + 1	AB194
A(LR) = TA	AB195
N(LR) = TN	AB196
EACT(LR) = TEA	AB197
DO 20 I=1,4	AB198
IF (SP(1,I) .EQ. EFFM) GO TO 19	AB199
IF (SP(1,I) .EQ. BLANK) GO TO 219	AB200
IF (LS .EQ. 0) GO TO 17	AB201
	AB202
	AB203
	AB204

C	MATCH INPUT SPECIES AGAINST INPUT SPECIES LIST	AB205
	DO 16 II=1,LS	AB206
	IF (DSPNM(II) .NE. DSP(I)) GO TO 16	AB207
	LSR(I,LR) = II	AB208
	GO TO 20	AB209
	16 CONTINUE	AB210
		AB211
C	MATCH INPUT SPECIES AGAINST MASTER SPECIES LIST	AB212
17	DO 18 II=1,75	AB213
	IF (DALSP(II) .NE. DSP(I)) GO TO 18	AB214
	LS = LS + 1	AB215
	LSR(I,LR) = LS	AB216
	SPNM(1,LS) = SP(1,I)	AB217
	SPNM(2,LS) = SP(2,I)	AB218
	MW(LS) = ALMW(II)	AB219
	ISS(LS) = II	AB220
	GO TO 20	AB221
	18 CONTINUE	AB222
C	ERROR MESSAGE - NO MATCH FOUND	AB223
	WRITE (6,102) (SP(K,I),K=1,2)	AB224
102	FORMAT (7H0(KINP),5X,54HTHE MASTER SPECIES LIST DOES NOT CONTAIN T	AB225
	*HE SPECIES ,2A4)	AB226
C **	RUN TERMINATED - ERROR IN INPUT REACTION LIST	AB227
	STOP	AB228
		AB229
	19 LSR(I,LR) = 0	AB230
	GO TO 20	AB231
		AB232
	219 LSR(I,LR) = -1	AB233
	20 CONTINUE	AB234
	GO TO 15	AB235
		AB236
	21 IF (ACTION .NE. NEW) GO TO 25	AB237
C	READ INERT SPECIES (4 PER CARD)	AB238
22	READ (LDAT,94) ((SP(K,I),K=1,2),I=1,4)	AB239
94	FORMAT (4(2A4,8X))	AB240
	DO 24 I=1,4	AB241
C	BLANK FIELD SIGNALS END OF INERT SPECIES LIST	AB242
	IF (SP(1,I) .EQ. BLANK) GO TO 25	AB243
C	SEARCH MASTER SPECIES LIST	AB244
	DO 23 II=1,75	AB245
	IF (DALSP(II) .NE. DSP(I)) GO TO 23	AB246
	LS = LS + 1	AB247
	SPNM(1,LS) = SP(1,I)	AB248
	SPNM(2,LS) = SP(2,I)	AB249
	MW(LS) = ALMW(II)	AB250
	ISS(LS) = II	AB251
	GO TO 24	AB252
	23 CONTINUE	AB253
C	ERROR MESSAGE - NO MATCH FOUND	AB254
	WRITE (6,102) (SP(K,I),K=1,2)	AB255
	NEXT = .TRUE.	AB256
	LS = LS + 1	AB257
	MW(LS) = 1.	AB258
	24 CONTINUE	AB259
	GO TO 22	AB260
		AB261
	25 IF (LS .EQ. LSOLD) GO TO 30	AB262

C	GET THERMODYNAMIC COEFFICIENTS FROM TAPE	AB263
	LSP = LSOLD + 1	AB264
	II = LSOLD	AB265
	READ (LTHM,98) TLOW,TMID,THI	AB266
26	READ (LTHM,97) (SPT(I),I=1,2)	AB267
	IF (SPT(1) .EQ. TAPEND) GO TO 29	AB268
	READ (LTHM,96) ((THMC(K,I),K=1,7),I=1,2)	AB269
	DO 28 I=LSP,LS	AB270
	IF (DSPNM(I) .NE. DSP(1)) GO TO 28	AB271
	DO 27 KK=1,2	AB272
	DO 27 K=1,7	AB273
27	TC(K,KK,I) = THMC(K,KK)	AB274
	II = II + 1	AB275
	IF (II .LT. LS) GO TO 26	AB276
	GO TO 230	AB277
28	CONTINUE	AB278
	GO TO 26	AB279
C	ERROR MESSAGE - END OF THERMO TAPE REACHED	AB280
29	WRITE (6,103)	AB281
103	FORMAT (7H0(KINP),5X,42HEND OF THERMO TAPE - NOT ALL SPECIES FOUND	AB282
	*)	AB283
	NEXT = .TRUE.	AB284
230	REWIND LTHM	AB285
		AB286
C	DETERMINE STOICHIOMETRIC COEFFICIENTS	AB287
30	LRP = LROLD + 1	AB288
	DO 31 I=1,LS	AB289
	DO 31 J=LRP,LR	AB290
	STOC = 0.	AB291
	IF (LSR(1,J) .EQ. I) STOC = STOC - 1.	AB292
	IF (LSR(2,J) .EQ. I) STOC = STOC - 1.	AB293
	IF (LSR(3,J) .EQ. I) STOC = STOC + 1.	AB294
	IF (LSR(4,J) .EQ. I) STOC = STOC + 1.	AB295
31	STOIC(I,J) = STOC	AB296
		AB297
		AB298
C	GET SPECIES ENTHALPY AT REFERENCE T	AB299
	TREF = 298.15	AB300
	CALL THRM (TREF,0.)	AB301
		AB302
	TRAL = TREF*1.987165	AB303
	DO 32 J=LRP,LR	AB304
	N1 = LSR(1,J)	AB305
	N2 = LSR(2,J)	AB306
	N3 = LSR(3,J)	AB307
	N4 = LSR(4,J)	AB308
C	COMPUTE HEAT OF REACTION	AB309
	DELH(J) = HRT(N3) - HRT(N2)	AB310
	IF (N1 .GT. 0) DELH(J) = DELH(J) - HRT(N1)	AB311
	IF (N4 .GT. 0) DELH(J) = DELH(J) + HRT(N4)	AB312
32	DELH(J) = DELH(J)*TRAL	AB313
		AB314
	LSP3 = LS + 3	AB315
C	RESET STANDARD OPTIONS	AB316
33	MOLEF = .TRUE.	AB317
	MMHG = .FALSE.	AB318
	NEWPRF = .FALSE.	AB319

C	INITIALIZE	AB320
	END = 0.	AB321
	DELP = 0.	AB322
	NTB = 0	AB323
	NPRTS = 0	AB324
	DO 34 I=1,50	AB325
34	APRINT(I) = 0.	AB326
	AREA = 0.	AB327
	MDOT = 0.	AB328
	P = 0.	AB329
	V = 0.	AB330
	RHO = 0.	AB331
	T = 0.	AB332
	HN = 0.	AB333
	ERRN = 0.	AB334
	NH = 0	AB335
	AVH = 0.	AB336
	JCV = 30	AB337
	KOUNT = 0	AB338
	DO 35 I=1,28	AB339
	RK(I) = 0.	AB340
35	E(I) = 0.	AB341
	I1 = 0	AB342
	I2 = 0	AB343
		AB344
C	READ NAME OF INDEPENDENT VARIABLE, NAME OF ASSIGNED VARIABLE,	AB345
C	INPUT UNITS, OUTPUT UNITS	AB346
	READ (LDAT,92) VERSI,VERSA,UNITI,UNITO	AB347
92	FORMAT (4(A4,6X))	AB348
	IF (VERSA .EQ. BLANK) VERSA = AREAV	AB349
		AB350
	IF (ACTION .NE. NEW) GO TO 80	AB351
C	INITIALIZE STEP SIZE LIMITS	AB352
	IF (VERSI .EQ. TIMEV) GO TO 78	AB353
	HMIN = 0.0001	AB354
	HMAX = 0.1000	AB355
	IPRCOD = 2	AB356
	GO TO 79	AB357
78	HMIN = 0.500E-07	AB358
	HMAX = 0.500E-04	AB359
	IPRCOD = 4	AB360
79	IF (VERSA .EQ. AREAV) IPRCOD = IPRCOD - 1	AB361
		AB362
C	READ INTEGRATION CONTROLS, PROFILE OPTIONS,	AB363
C	PRINT OPTIONS, SPECIALTY SWITCHES	AB364
80	READ (LDAT,PROB)	AB365
		AB366
	IF (.NOT. ALLM1) GO TO 36	AB367
	DO 77 I=1,25	AB368
	DO 77 J=1,30	AB369
77	M(I,J) = 1.	AB370
	GO TO 40	AB371
C	READ THIRD BODY RATIOS	AB372
36	READ (LDAT,91) ((SP(K,I),K=1,2),I=1,4),((SPP(K,I),K=1,2),TBR(I),	AB373
	* I=1,3)	AB374
91	FORMAT (2(2A4,1X),1X,2(1X,2A4),1X,3(2A4,F6.4))	AB375
C	BLANK CARD SIGNALS END OF THIRD BODY RATIO LIST	AB376
	IF (SP(1,2) .EQ. BLANK) GO TO 40	AB377

C	SEARCH INPUT REACTION LIST	AB378
	DO 39 J=1,LR	AB379
	N1 = LSR(1,J)	AB380
	N2 = LSR(2,J)	AB381
	N3 = LSR(3,J)	AB382
	IF (N1 .EQ. 0) N1 = 26	AB383
	IF (N1 .LT. 0) N1 = 27	AB384
	IF (DSPNM(N1) .NE. DSP(1) .OR. DSPNM(N2) .NE. DSP(2) .OR. DSPNM(N3	AB385
	*) .NE. DSP(3)) GO TO 39	AB386
	DO 38 I=1,3	AB387
	IF (SPP(1,I) .EQ. BLANK) GO TO 38	AB388
C	SEARCH INPUT SPECIES LIST	AB389
	DO 37 II=1,LS	AB390
	IF (DSPNM(II) .NE. DSPP(I)) GO TO 37	AB391
	M(II,J) = TBR(I)	AB392
	GO TO 38	AB393
	37 CONTINUE	AB394
C	ERROR MESSAGE - NO MATCH FOUND	AB395
	WRITE (6,104) (SPP(K,I),K=1,2)	AB396
104	FORMAT (7H0(KINP),5X,53HTHE INPUT SPECIES LIST DOES NOT CONTAIN TH	AB397
	*E SPECIES ,2A4)	AB398
	NEXT = .TRUE.	AB399
	38 CONTINUE	AB400
	GO TO 36	AB401
	39 CONTINUE	AB402
C	ERROR MESSAGE - NO MATCH FOUND	AB403
	WRITE (6,101) ((SP(K,I),K=1,2),I=1,4)	AB404
	NEXT = .TRUE.	AB405
	GO TO 36	AB406
		AB407
C	GET INITIAL CONDITIONS	AB408
	40 CALL INIT (ISS,MMHG,MOLEF)	AB409
		AB410
C	READ SPECIES TO BE NEGLECTED FROM ERROR CONSIDERATIONS (4 PER CARD)	AB411
	41 READ (LDAT,94) ((SP(K,I),K=1,2),I=1,4)	AB412
	DO 43 I=1,4	AB413
C	BLANK FIELD SIGNALS END OF NEGLECTED SPECIES LIST	AB414
	IF (SP(1,I) .EQ. BLANK) GO TO 44	AB415
C	SEARCH INPUT SPECIES LIST	AB416
	DO 42 II=1,LS	AB417
	IF (DSPNM(II) .NE. DSP(I)) GO TO 42	AB418
	I1 = I1 + 1	AB419
	NEGL(I1) = II	AB420
	GO TO 43	AB421
	42 CONTINUE	AB422
C	ERROR MESSAGE - NO MATCH FOUND	AB423
	WRITE (6,104) (SP(K,I),K=1,2)	AB424
	NEXT = .TRUE.	AB425
	43 CONTINUE	AB426
	GO TO 41	AB427
	44 IT = I1	AB428
		AB429
C	CHECK INPUT COMPOSITION	AB430
	CSUM = 0.	AB431
	DO 47 I=1,LS	AB432
	47 CSUM = CSUM + C(I)	AB433
	IF (ABS(1.-CSUM) .LE. .001) GO TO 48	AB434
	WRITE (6,105) CSUM, ((SPNM(K,I),K=1,2),C(I),I=1,LS)	AB435

105	FORMAT (7H0(KINP),5X,33HINVALID INPUT COMPOSITION SUM = ,F11.6//	AB436
	* (12X,2A4,E20.5))	AB437
	NEXT = .TRUE.	AB438
	RETURN	AB439
C	SET INITIAL STEP SIZE	AB440
48	HI = HINT	AB441
	IF (HINT .EQ. 0.) HI = HMIN	AB442
		AB443
		AB444
	IF (ITPSZ .GT. 2) GO TO 53	AB445
	IF (ITPSZ .EQ. 1 .AND. NTB .EQ. 0) GO TO 53	AB446
	IF (NTB .NE. 0) NT = NTB	AB447
	CONV = 1.	AB448
	CON2 = 1.	AB449
	IF (VERSA .NE. AREAV) GO TO 203	AB450
	XU = CU	AB451
	AU(1) = CUA(1)	AB452
	AU(2) = CUA(2)	AB453
C	CONVERT AREA PROFILE TO INTERNAL UNITS	AB454
	IF (UNITI .NE. FPS) GO TO 201	AB455
	XU = FU	AB456
	AU(1) = FUA(1)	AB457
	AU(2) = FUA(2)	AB458
	CONV = 30.48	AB459
	GO TO 202	AB460
201	IF (UNITI .NE. SI) GO TO 206	AB461
	XU = SU	AB462
	AU(1) = SUA(1)	AB463
	AU(2) = SUA(2)	AB464
	CONV = 100.	AB465
202	CON2 = CONV*CONV	AB466
	GO TO 206	AB467
		AB468
203	XU = CU	AB469
	AU(1) = CUP2(1)	AB470
	AU(2) = CUP2(2)	AB471
C	CONVERT PRESSURE PROFILE TO INTERNAL UNITS	AB472
	IF (UNITI .NE. FPS) GO TO 204	AB473
	XU = FU	AB474
	AU(1) = FUP(1)	AB475
	AU(2) = FUP(2)	AB476
	CONV = 30.48	AB477
	CON2 = 1./2116.2	AB478
	GO TO 205	AB479
204	IF (UNITI .NE. SI) GO TO 205	AB480
	XU = SU	AB481
	AU(1) = SUP(1)	AB482
	AU(2) = SUP(2)	AB483
	CONV = 100.	AB484
	CON2 = 1./1.01325E+05	AB485
205	IF (.NOT. MMHG) GO TO 206	AB486
	AU(1) = CUP1(1)	AB487
	AU(2) = CUP1(2)	AB488
	CON2 = 1./760.	AB489
		AB490
206	IF (VERSI .EQ. TIMEV) CONV = 1	AB491
	IF (ITPSZ .EQ. 2) GO TO 208	AB492
	DO 207 I=1,NTB	AB493
	CXTB(I) = XTB(I)*CONV	AB494
207	CATB(I) = ATB(I)*CON2	AB495
	GO TO 53	AB496
208	DO 209 I=1,4	AB497

209	CN(I) = CX(I)*CON2	AB498
		AB499
53	IF ((NPRNTS .NE. 0) .OR. (DELP .NE. 0.) .OR. (END .NE. 0.)) NEWPRT	AB500
	* = .TRUE.	AB501
	IF (.NOT. NEWPRT) GO TO 59	AB502
	IF (END .NE. 0.) UNCEND = END	AB503
C	PREPARE PRINT STATIONS	AB504
	IF (EVSTEP) GO TO 59	AB505
	IF (NPRNTS .NE. 0) GO TO 57	AB506
	IF (DELP .NE. 0.) GO TO 54	AB507
	DELP = (UNCEND - IVAR)/24.9999	AB508
54	PRINT(1) = IVAR + DELP	AB509
	DO 55 I=2,50	AB510
	PRINT(I) = PRINT(I-1) + DELP	AB511
	IF (PRINT(I) .GE. UNCEND) GO TO 56	AB512
55	CONTINUE	AB513
56	NP = I	AB514
	PRINT(NP) = UNCEND	AB515
	GO TO 59	AB516
		AB517
57	NP = NPRNTS	AB518
	IF (APRINT(1) .EQ. 0.) GO TO 59	AB519
	CONV = 1.	AB520
	IF (IPRCOD .EQ. 2 .OR. IPRCOD .EQ. 4) GO TO 210	AB521
	IF (UNITI .EQ. FPS) CONV = 30.48	AB522
	IF (UNITI .EQ. SI) CONV = 100.	AB523
	CON2 = CONV*CONV	AB524
	GO TO 213	AB525
210	CON2 = 1.	AB526
	IF (UNITI .NE. FPS) GO TO 211	AB527
	CONV = 30.48	AB528
	CON2 = 1./2116.2	AB529
	GO TO 212	AB530
211	IF (UNITI .NE. SI) GO TO 212	AB531
	CONV = 100.	AB532
	CON2 = 1./1.01325E+05	AB533
212	IF (MMHG) CON2 = 1./760.	AB534
213	IF (VERSI .EQ. TIMEV) CONV = 1.	AB535
	CALL CUBS (CATB,CXTB,NT)	AB536
	DO 58 I=1,NPRNTS	AB537
	APRINT(I) = APRINT(I)*CON2	AB538
	CALL CIMP (APRINT(I),PRINT(I),DUM1,DUM2)	AB539
58	PRINT(I) = PRINT(I)/CONV	AB540
		AB541
59	IF (ITPSZ .EQ. 1) CALL CUBS (CXTB,CATB,NT)	AB542
		AB543
	IF (UNITI .NE. FPS) GO TO 63	AB544
C	CONVERT FROM FPS UNITS TO INTERNAL (CGS) UNITS	AB545
	IF (VERSI .NE. TIMEV) GO TO 60	AB546
	DVAR = DVAR*30.48	AB547
	GO TO 61	AB548
60	IVAR = IVAR*30.48	AB549
61	IF (MMHG) P = P*2.7845	AB550
	P = P/2116.2	AB551
	AREA = APEA*929.0304	AB552
	MDOT = MDOT*453.59237	AB553
	V = V*30.48	AB554
	RHO = RHO/62.43	AB555
	T = T/1.8	AB556
	IF ((.NOT. NEWPRT) .OR. VERSI .EQ. TIMEV) GO TO 68	AB557
	CEND = UNCEND*30.48	AB558
	DO 62 I=1,NP	AB559

62 PRINT (I) = PRINT (I) * 30.48	AB560
GO TO 68	AB561
63 IF (UNITI .NE. SI) GO TO 67	AB562
C CONVERT FROM SI UNITS TO INTERNAL (CGS) UNITS	AB563
IF (VERSI .NE. TIMEV) GO TO 64	AB564
DVAR = DVAR*100.	AB565
GO TO 65	AB566
64 IVAR = IVAR*100.	AB567
65 IF (MMHG) P = P*133.3224	AB568
P = P/1.01325E+05	AB569
AREA = AREA*10000.	AB570
MDOT = MDOT*1000.	AB571
V = V*100.	AB572
RHC = RHO*.001	AB573
IF ((.NOT. NEWPRT) .OR. VERSI .EQ. TIMEV) GO TO 68	AB574
CEND = UNCEND*100.	AB575
DO 66 I=1,NP	AB576
66 PRINT (I) = PRINT (I) * 100.	AB577
GO TO 68	AB578
67 CEND = UNCEND	AB579
IF (MMHG) P = P/760.	AB580
68 MIXMW = 0.	AB581
IF (.NOT. MOLEF) GO TO 71	AB582
C MOLE FRACTION TO MOLES (I) / MASS (MIXTURE)	AB583
DO 69 I=1,LS	AB584
69 MIXMW = MIXMW + C (I) * MW (I)	AB585
DO 70 I=1,LS	AB586
70 SIGMA (I) = C (I) / MIXMW	AB587
GO TO 73	AB588
C MASS FRACTION TO MOLES (I) / MASS (MIXTURE)	AB589
71 DO 72 I=1,LS	AB590
SIGMA (I) = C (I) / MW (I)	AB591
72 MIXMW = MIXMW + SIGMA (I)	AB592
MIXMW = 1. / MIXMW	AB593
C UNIVERSAL GAS CONSTANT IN ATM-CC/MOLE-DEG K	AB594
73 RR = 82.056	AB595
C UNIVERSAL GAS CONSTANT IN ERGS/MOLE-DEG K	AB596
R = 8.3143E+07	AB597
IF (M2 .EQ. 0. .AND. .NOT. (CCMBUS .OR. SHOCK)) GO TO 81	AB598
CALL THRM (T, 1.)	AB599
CPR0 = 0.	AB600
DO 74 I=1,LS	AB601
74 CPR0 = CPR0 + CPR (I) * SIGMA (I)	AB602
GAMMA = CPR0 / (CPR0 - 1. / MIXMW)	AB603
IF (V .NE. 0.) GO TO 81	AB604
V = SQRT (M2 * R / MIXMW * GAMMA * T)	AB605
81 IF (P .EQ. 0.) GO TO 82	AB606
RHO = P * MIXMW / (RR * T)	AB607
GO TO 75	AB608
82 IF (RHO .EQ. 0.) GO TO 83	AB609
P = RHO * RR * T / MIXMW	AB610
GO TO 75	AB611
	AB612
	AB613
	AB614
	AB615
	AB616
	AB617
	AB618
	AB619

83 IF (IPRCOD .GT. 2) GO TO 84	AB620
X = IVAR	AB621
IF (VERSI .EQ. TIMEV) X = DVAR	AB622
CALL CINP (X,AVAR,DUM1,DUM2)	AB623
GO TO 85	AB624
84 TIME = DVAR	AB625
IF (VERSI .EQ. TIMEV) TIME = IVAR	AB626
CALL CINP (TIME,AVAR,DUM1,DUM2)	AB627
85 IF (VERSA .EQ. AREAV) GO TO 86	AB628
P = AVAR	AB629
GO TO 81	AB630
86 AREA = AVAR	AB631
RHO = MDOT/(AREA*V)	AB632
GO TO 82	AB633
75 IF (MDOT .EQ. 0.) MDOT = RHO*ARFA*V	AB634
IF (.NOT. (COMBUS .OR. SHOCK)) RETURN	AB635
HRO = 0.	AB636
DO 76 I=1,LS	AB637
76 HRO = HRO + HRT(I)*SIGMA(I)	AB638
HRO = HRO*T	AB639
M2 = V/R*V/T*MIXMW/GAMMA	AB640
C EQUILIBRIUM COMBUSTION	AB641
IF (COMBUS) CALL COMB	AB642
	AB643
C EQUILIBRIUM AND FROZEN SHOCK	AB644
IF (SHOCK) CALL SHOK	AB645
	AB646
RETURN	AB647
END	AB648
\$IBFTC INITT DECK	AB649
SUBROUTINE INIT (ISS,MMHGS,MOLEFS)	AB650
	AB651
C READ INITIAL CONDITIONS	AC001
LOGICAL MMHG,MOLEF,MMHGS,MOLEFS	AC002
	AC003
REAL IVAR,MDOT,M2,MACH	AC004
REAL N,NF,NF2,NF3,NH2,NH3,NO,NO2,N2,N2H4,N2O,N2O4,NE,KR,NH,NOP	AC005
	AC006
DIMENSION ISS(25),TINP(75)	AC007
COMMON/LTUS/LTHM,LDAT	AC008
COMMON/OPTS/VERSI,TIMEV,DUM1(6)	AC009
COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,CONC(25),LS,DUM2(2)	AC010
COMMON/NECC/DUM3(2),M2,DUM4(3)	AC011
COMMON/FAKE/	AC012
1 AR,B,BF,BF2,BF3,BH,BH2,BH3,BO,BOF,BOF2,BO2,B2O3,BR,BR2,C,CF,CF2,	AC013
2 CH,CH2,CH3,CH4,CN,CO,CO2,C2F2,C2H,C2H2,C2H4,C2N,CL,CLF,CLF3,CL2,	AC014
3 F,F2,H,HCN,HCL,HF,HO2,H2,H2O,H2O2,HE,N,NF,NF2,NF3,NH2,NH3,NO,NO2,	AC015
4 N2,N2H4,N2C,N2O4,NE,O,OH,O2,HNO,KR,XE,NH,HCO,CH2O,NOP,OP,OM,O2M,E	AC016
	AC017
EQUIVALENCE (TINP(1),AR)	AC018
	AC019
NAMELIST/START/X,AREA,MDOT,P,TIME,V,RHO,T, MACH, MMHG,MOLEF,	AC020
1 AR,B,BF,BF2,BF3,BH,BH2,BH3,BO,BOF,BOF2,BO2,B2O3,BR,BR2,C,CF,CF2,	AC021
2 CH,CH2,CH3,CH4,CN,CO,CO2,C2F2,C2H,C2H2,C2H4,C2N,CL,CLF,CLF3,CL2,	AC022
3 F,F2,H,HCN,HCL,HF,HO2,H2,H2O,H2O2,HE,N,NF,NF2,NF3,NH2,NH3,NO,NO2,	AC023
4 N2,N2H4,N2C,N2O4,NE,O,OH,O2,HNO,KR,XE,NH,HCO,CH2O,NOP,OP,OM,O2M,E	AC024
	AC025
	AC026
	AC027
	AC028
	AC029

X = 0.	AC030
TIME = 0.	AC031
MACH = 0.	AC032
DO 1 II=1,75	AC033
1 TNP(II) = 0.	AC034
MMHG = MMHGS	AC035
MOLEF = MOLEFS	AC036
READ (LDAT,START)	AC037
	AC038
MMHGS = MMHG	AC039
MOLEFS = MOLEF	AC040
IF (VERSI .EQ. TIMEV) GO TO 2	AC041
IVAR = X	AC042
DVAR = TIME	AC043
GO TO 3	AC044
2 IVAR = TIME	AC045
DVAR = X	AC046
	AC047
3 M2 = MACH*MACH	AC048
DO 4 II=1,LS	AC049
JJ = ISS(II)	AC050
4 CONC(II) = TNP(JJ)	AC051
	AC052
RETURN	AC053
END	AC054
\$IEFTC CDIMAG DECK	AC055
SUBROUTINE CIMAGE	AD001
	AD002
C THIS ROUTINE READS EACH DATA CARD, PRINTS A CARD IMAGE, AND STORES	AD003
C THE IMAGE FOR LATER FORMATTED INPUT	AD004
	AD005
DIMENSION CARD(20)	AD006
	AD007
COMMON/LTUS/LTHM,LDAT	AD008
	AD009
EQUIVALENCE (WORD,CARD)	AD010
	AD011
DATA FINIS,PLANK/4HFINI,1H /	AD012
	AD013
READ (5,101) CARD	AD014
101 FORMAT (20A4)	AD015
REWIND LDAT	AD016
	AD017
WRITE (6,100)	AD018
100 FORMAT (1H1,56X,18H** DATA CARDS **//37X,1H1,9X,1H2,9X,1H3,9X,	AD019
* 1H4,9X,1H5,9X,1H6,9X,1H7,9X,1H8/24X,5HCC 1,8X,8(1H0,9X)//)	AD020
GO TO 2	AD021
	AD022
1 READ (5,101) CARD	AD023
2 DO 3 I=1,20	AD024
IF (CARD(I) .NE. BLANK) GO TO 4	AD025
3 CONTINUE	AD026
WRITE (6,102)	AD027
102 FORMAT (60X,16H- BLANK CARD -)	AD028
GO TO 5	AD029
4 WRITE (6,103) CARD	AD030
103 FORMAT (28X,20A4)	AD031
IF (WORD .EQ. FINIS) GO TO 6	AD032
5 WRITE (LDAT,101) CARD	AD033
GO TO 1	AD034
	AD035

```

6 REWIND LDAT
RETURN
END
$IEFTC NAMBLK DECK
BLOCK DATA

C ALPHANUMERIC DATA FOR TESTING AND OUTPUT

COMMON/LTUS/LTHM,LDAT
COMMON/OPTS/DUM1,TIME,DUM2,AREA,DUM3(4)
COMMON/SPEC/SNAM(2,3),DUM4(2,25),EFFM(2),BLANK(2),DUM5(25,62)
COMMON/KOUT/DUM6(54),FPS,SI,DUM7

C LOGICAL TAPE UNIT ASSIGNMENTS
DATA LTHM,LDAT/4,7/

C ALPHANUMERIC DATA
DATA TIME,AREA/4HTIME,4HAREA/
DATA SNAM,EFFM,BLANK/1HV,1H,3HRHO,1H,1HT,1H,1HM,1H,1H,1H /
DATA FPS,SI/3HFPS,2HSI/

END
$IEFTC BLCK DECK
BLOCK DATA

C SPECIES NAMES AND MOLECULAR WEIGHTS

COMMON/SNMW/ALSP(2,75),ALMW(75)

DATA ALSP/
* 4HAR ,4H , 4HB ,4H , 4HBF ,4H , 4HBF2 ,4H ,
* 4HBF3 ,4H , 4HBH ,4H , 4HBH2 ,4H , 4HBH3 ,4H ,
* 4HBO ,4H , 4HBOF ,4H , 4HBOF2 ,4H , 4HBO2 ,4H ,
* 4HB2O3 ,4H , 4HBR ,4H , 4HBP2 ,4H , 4HC ,4H ,
* 4HCF ,4H , 4HCF2 ,4H , 4HCH ,4H , 4HCH2 ,4H ,
* 4HCH3 ,4H , 4HCH4 ,4H , 4HCN ,4H , 4HCO ,4H ,
* 4HCO2 ,4H , 4HC2F2 ,4H , 4HC2H ,4H , 4HC2H2 ,4H ,
* 4HC2H4 ,4H , 4HC2N ,4H , 4HCL ,4H , 4HCLF ,4H ,
* 4HCLF3 ,4H , 4HCL2 ,4H , 4HF ,4H , 4HF2 ,4H ,
* 4HH ,4H , 4HHCN ,4H , 4HHCL ,4H , 4HHF ,4H ,
* 4HHO2 ,4H , 4HH2 ,4H , 4HH2O ,4H , 4HH2O2 ,4H ,
* 4HHE ,4H , 4HN ,4H , 4HNF ,4H , 4HNF2 ,4H ,
* 4HNF3 ,4H , 4HNH2 ,4H , 4HNH3 ,4H , 4HNO ,4H ,
* 4HNO2 ,4H , 4HN2 ,4H , 4HN2H4 ,4H , 4HN2O ,4H ,
* 4HN2O4 ,4H , 4HNE ,4H , 4HO ,4H , 4HOF ,4H ,
* 4HO2 ,4H , 4HHNO ,4H , 4HKP ,4H , 4HXF ,4H ,
* 4HNH ,4H , 4HHCO ,4H , 4HCH2O ,4H , 4HNO+ ,4H ,
* 4HO- ,4H , 4HO+ ,4H , 4HO2- ,4H , 4HE ,4H ,
* 6*0./

DATA ALMW/
* 39.948, 10.811, 29.809, 48.808,
* 67.806, 11.819, 12.827, 13.835,
* 26.810, 45.807, 64.807, 42.810,
* 69.620, 79.909, 159.82, 12.0112,
* 31.010, 50.008, 13.019, 14.027,
* 15.035, 16.043, 26.018, 28.011,
* 44.010, 62.019, 25.030, 26.038,
* 28.054, 38.029, 35.453, 54.451,
* 92.448, 70.906, 18.9984, 37.997,
* 1.00797, 27.026, 36.461, 20.006,

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AD036
AD037
AD038
AD039

AE001
AE002
AE003
AE004
AE005
AE006
AE007
AE008
AE009
AE010
AE011
AE012
AE013
AE014
AE015
AE016
AE017
AE018

AF001
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AF018
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AF021
AF022
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AF024
AF025
AF026
AF027
AF028
AF029
AF030
AF031
AF032
AF033
AF034
AF035
AF036
AF037
AF038

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* 33.005,	2.0159,	18.014,	34.014,	AF039
* 4.0026,	14.007,	33.005,	52.004,	AF040
* 71.002,	16.023,	17.031,	30.006,	AF041
* 46.006,	28.013,	32.045,	44.012,	AF042
* 92.009,	20.183,	15.9994,	17.007,	AF043
* 31.997,	31.014,	83.800,	131.30,	AF044
* 15.015,	29.0186,	30.026,	30.00555,	AF045
* 15.99995,	15.99885,	31.99935,	5.48597E-04,	AF046
* 3*0./				AF047
				AF048
				AF049
END				
\$IBFTC COMBB DECK				
SUBROUTINE COMB				AG001
				AG002
C EQUILIBRIUM COMBUSTION CALCULATIONS				AG003
				AG004
DOUBLE PRECISION EN,ENLN,DELN				AG005
				AG006
LOGICAL TP,HP				AG007
				AG008
COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT				AG009
COMMON/SPEC/DUM1(6),SPNM(2,27),DUM2(25,62)				AG010
COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)				AG011
COMMON/INDX/TP,HP,DUM3(6)				AG012
COMMON/MISC/TT,PP,CPRO,HRO,ENN,DUM4(32)				AG013
				AG014
TP = .FALSE.				AG015
HP = .TRUE.				AG016
				AG017
CALL ELEMNT (LS,SPNM,SIGMA)				AG018
ENI = 0.1/FLOAT(LS)				AG019
ENIL = ALOG(ENI)				AG020
DO 3 I=1,LS				AG021
EN(I) = ENI				AG022
3 ENLN(I) = ENIL				AG023
ENN = 0.1				AG024
				AG025
TT = 3800.				AG026
PP = P				AG027
CALL EQLBRM				AG028
				AG029
CALL Ecout				AG030
				AG031
RETURN				AG032
END				AG033
\$IBFTC SHOKK DECK				
SUBROUTINE SHOK				AH001
				AH002
C EQUILIBRIUM AND FROZEN SHOCK CALCULATIONS				AH003
				AH004
DOUBLE PRECISION EN,FNLN,DELN				AH005
DOUBLE PRECISION DLVTP,DLVPT				AH006
				AH007
LOGICAL TP,HP,EQL				AH008
				AH009
REAL MIXMW				AH010
				AH011
COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT				AH012
COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R				AH013
COMMON/SPEC/DUM1(6),SPNM(2,27),DUM2(25,62)				AH014
COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)				AH015
COMMON/POINTS/DLVTP,DLVPT,GAM,W				AH016
COMMON/INDX/TP,HP,DUM3(6)				AH017
COMMON/MISC/TT,PP,CPRO,HRO,ENN,DUM4(32)				AH018
				AH019

C	INITIALIZE	AH020
	TP = .TRUE.	AH021
	HP = .FALSE.	AH022
		AH023
C	EQUILIBRIUM SHOCK	AH024
	CALL ELEMNT (LS,SPNM,SIGMA)	AH025
	GAM = GAMMA	AH026
	ENI = 0.1/FLOAT(LS)	AH027
	ENIL = ALOG(ENI)	AH028
	DO 2 I=1,LS	AH029
	EN(I) = ENI	AH030
	2 ENLN(I) = ENIL	AH031
	ENN = 0.1	AH032
	EQL = .TRUE.	AH033
	CALL SHOCKS (EQL)	AH034
	CALL ESOUT	AH035
		AH036
C	FROZEN SHOCK	AH037
	WM = MIXMW	AH038
	DLVTP = 1.D0	AH039
	DLVPT = -1.D0	AH040
	GAM = GAMMA	AH041
	DO 3 I=1,LS	AH042
	3 EN(I) = SIGMA(I)	AH043
	EQL = .FALSE.	AH044
	CALL SHOCKS (EQL)	AH045
	CALL FSOUT	AH046
		AH047
	RETURN	AH048
	END	AH049
	\$IBFTC SHCKS DECK	
	SUBROUTINE SHOCKS (EQL)	AI001
		AI002
C	SHOCK EQUATIONS	AI003
		AI004
	DOUBLE PRECISION A,Y,AA	AI005
	DOUBLE PRECISION SIGMA,ENLN,DELN	AI006
	DOUBLE PRECISION DLVTP,DLVPT	AI007
		AI008
	LOGICAL EQL,NEXT	AI009
		AI010
	REAL MIXMW,M2	AI011
		AI012
	DIMENSION A(2,3),Y(3)	AI013
		AI014
	COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,DUM1(25),LS,LSP3,NEXT	AI015
	COMMON/NECC/RR,MIXMW,M2,DUM2,TCPR,R	AI016
	COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)	AI017
	COMMON/SPECES/SIGMA(25),ENLN(25),DELN(25),AAA(15,25)	AI018
	COMMON/POINTS/DLVTP,DLVPT,GAMMA,WM	AI019
	COMMON/MISC/TT,PP,CPR0,HRO,DUM3(33)	AI020
		AI021
C	INITIAL ESTIMATE OF PRESSURE AND TEMPERATURE RATIOS	AI022
	P21 = (2.*GAMMA*M2 - GAMMA + 1.)/(GAMMA + 1.)	AI023
	T21 = P21*(2./M2 + GAMMA - 1.)/(GAMMA + 1.)	AI024
	IF (EQL .AND. T*T21 .GT. 2000.) T21 = 0.7*T21 + 600./T	AI025
		AI026
	CONST = MIXMW*V/R*V/T	AI027
	P21L = ALOG(P21)	AI028
	T21L = ALOG(T21)	AI029
		AI030

```

C      ITERATE ON PRESSURE AND TEMPERATURE RATIOS
      DO 4 K=1,8
      PP = P21*P
      TT = T21*T
      IF (EQL) CALL EQLBRM
      CALL THRM (TT,1.)
      IF (NEXT) GO TO 5
      TCPR = 0.
      THR = 0.
      DO 2 I=1,LS
      TCPR = TCPR + CPR(I)*SIGMA(I)
2     THR = THR + HRT(I)*SIGMA(I)
      THR = THR*TT
      RHO12 = T21/P21*MIXMW/MM

      AA = RHO12*CONST
      A(1,1) = -AA*DLVPT - P21
      A(1,2) = -AA*DLVTP
      A(1,3) = P21 - 1. + CONST*(RHO12 - 1.)
      AA = (V*RHO12)**2/R
      A(2,1) = -AA*DLVPT + TT*(DLVTP - 1.)/WM
      A(2,2) = -AA*DLVTP - TT*TCPR
      A(2,3) = THR - HRO - V*V*(1. - RHO12*RHO12)/(2.*R)

      Y(3) = A(1,1)*A(2,2) - A(1,2)*A(2,1)
      Y(2) = (A(1,1)*A(2,3) - A(2,1)*A(1,3))/Y(3)
      Y(1) = -(A(1,3)*A(2,2) - A(2,3)*A(1,2))/Y(3)

      Y1 = DABS(Y(1))
      Y2 = DABS(Y(2))
      IF (Y2 .GT. Y1) Y1 = Y2
      IF (Y1 .LT. 0.5E-04) RETURN
      Y1 = Y1/0.4054652
      IF (Y1 .LE. 1.) GO TO 3
      Y(1) = Y(1)/Y1
      Y(2) = Y(2)/Y1

3     P21L = P21L + Y(1)
      T21L = T21L + Y(2)
      P21 = EXP(P21L)
      T21 = EXP(T21L)
4     CONTINUE

5     IF (.NOT. EQL) GO TO 6
      WRITE (6,100)
100    FORMAT (9H0(SHOCKS),5X,36HEQUILIBRIUM SHOCK CALCULATION FAILED)
      NEXT = .FALSE.
      RETURN

6     WRITE (6,101)
101    FORMAT (9H0(SHOCKS),5X,31HFROZEN SHOCK CALCULATION FAILED)
      NEXT = .TRUE.
      RETURN

      END
$IEFTC ELMENT DECK
      SUBROUTINE ELEMNT (LS,DSPEC,SIGMA)

C      COLLECT ELEMENT DATA FOR EQUILIBRIUM SHOCK OR COMBUSTION

      DOUBLE PRECISION DSPEC,DSP
      DOUBLE PRECISION EN,ENLN,DELN

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AI031
AI032
AI033
AI034
AI035
AI036
AI037
AI038
AI039
AI040
AI041
AI042
AI043
AI044
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AI071
AI072
AI073
AI074
AI075
AI076
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AI078
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AI080
AI081
AI082
AI083
AI084
AI085
AJ001
AJ002
AJ003
AJ004
AJ005
AJ006
AJ007

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DIMENSION DSPEC(25),SIGMA(25),SP(2),LMT(4),SUBS(4)	AJ008
COMMON/LTUS/LTHM,LDAT	AJ009
COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)	AJ010
COMMON/MISC/DUM1(7),LLMT(15),B0(15)	AJ011
COMMON/INDX/TP,HP,NLM,NS,IQ1,DUM2(3)	AJ012
	AJ013
	AJ014
EQUIVALENCE (DSP,SP(1))	AJ015
	AJ016
IF (LS .EQ. NS) GO TO 10	AJ017
C CONSTRUCT LIST OF ELEMENTS PRESENT	AJ018
READ (LTHM,99) DUMMY	AJ019
NSP = NS + 1	AJ020
2 READ (LTHM,99) (SP(K),K=1,2),(LMT(K),SUBS(K),K=1,4),DUMM1,DUMM2,	AJ021
* DUMM3	AJ022
99 FORMAT (2A4,16X,4(A2,F3.0)/A1/A1/A1)	AJ023
DO 8 I=NSP,LS	AJ024
IF (DSPEC(I) .NE. DSP) GO TO 8	AJ025
DO 3 L=1,15	AJ026
3 A(L,I) = 0.	AJ027
IF (NLM .NE. 0) GO TO 4	AJ028
NLM = 1	AJ029
LLMT(NLM) = LMT(1)	AJ030
4 DO 6 K=1,4	AJ031
IF (SUBS(K) .EQ. 0.) GO TO 7	AJ032
DO 5 L=1,NLM	AJ033
IF (LLMT(L) .NE. LMT(K)) GO TO 5	AJ034
A(L,I) = SUBS(K)	AJ035
GO TO 6	AJ036
5 CONTINUE	AJ037
NLM = NLM + 1	AJ038
LLMT(NLM) = LMT(K)	AJ039
A(NLM,I) = SUBS(K)	AJ040
6 CONTINUE	AJ041
7 NS = NS + 1	AJ042
IF (NS .LT. LS) GO TO 2	AJ043
GO TO 9	AJ044
8 CONTINUE	AJ045
GO TO 2	AJ046
9 REWIND LTHM	AJ047
	AJ048
	AJ049
	AJ050
C COMPUTE ELEMENT CONCENTRATION IN GM-ATOMS/GM	AJ051
10 DO 11 L=1,NLM	AJ052
B0(L) = 0.	AJ053
DO 11 I=1,LS	AJ054
11 B0(L) = B0(L) + A(L,I)*SIGMA(I)	AJ055
IQ1 = NLM + 1	AJ056
	AJ057
RETURN	AJ058
END	
\$IBFTC EQUIL DECK	AK001
SUBROUTINE FQLBRM	AK002
C CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES	AK003
	AK004
DOUBLE PRECISION G,X,SUM	AK005
DOUBLE PRECISION EN,ENLN,DELN	AK006
DOUBLE PRECISION DLVTP,DLVPT	AK007
	AK008
LOGICAL CONVG,ISING,LOGV,TP,NEXT	AK009
	AK010

DIMENSION PROW(18)	AK011
COMMON/POINTS/DLVTP,DLVPT,GAMMA,WM	AK012
COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)	AK013
COMMON/MISC/TT,PP,CPR0,HSUB0,ENN,SUMN,ENNL,LLMT(15),B0(15)	AK014
COMMON/INDX/TP,HP,NLM,NS,IQ1,CONVG,KMAT,IMAT	AK015
COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPP(25)	AK016
COMMON/MATX/G(28,28),X(28)	AK017
COMMON/NECC/DUM1(4),CPSUM,DUM2	AK018
COMMON/COND/DUM3(35),NEXT	AK019
	AK020
C INITIALIZE	AK021
SMALNO = 1.0E-06	AK022
SMNOL = -13.815511	AK023
SIZE = 18.5	AK024
SIZEF = 0.	AK025
CONVG = .FALSE.	AK026
ISING = .FALSE.	AK027
LOGV = .FALSE.	AK028
ITN = 35	AK029
ITNUMB = ITN	AK030
TLN = ALOG(TT)	AK031
TM = ALOG(PP/FNN)	AK032
ENNL = ALOG(ENN)	AK033
CALL THRM (TT,1.)	AK034
CPSUM = 0.	AK035
DO 2 I=1,NS	AK036
2 CPSUM = CPSUM + CPR(I)*EN(I)	AK037
	AK038
	AK039
C BEGIN ITERATION	AK040
43 CALL MATRIX	AK041
NUMB = ITN- (ITNUMB - 1)	AK042
IQ2 = IQ1 + 1	AK043
IF (.NOT. CONVG) GO TO 67	AK044
IF (LOGV) GO TO 63	AK045
DO 182 L=1,NLM	AK046
182 PROW(L) = G(IQ1,L)	AK047
GO TO 72	AK048
	AK049
C LOGV = .TRUE. --- SET UP MATRIX TO SOLVE FOR DLVPT	AK050
63 G(IQ1,IQ2) = ENN	AK051
IQ = IQ1 - 1	AK052
DO 777 I=1,IQ	AK053
777 G(I,IQ2) = G(I,IQ1)	AK054
72 IMAT = IMAT - 1	AK055
67 ITST = IMAT	AK056
CALL GAUSS	AK057
IF (ITST .NE. IMAT) GO TO 774	AK058
IF (.NOT. CONVG) GO TO 85	AK059
IF (LOGV) GO TO 171	AK060
SUM = 0.	AK061
DO 175 L=1,NLM	AK062
175 SUM = SUM + PROW(L)*X(L)	AK063
DLVTP = 1. + (G(IQ2,IQ1) - SUM)/ENN - X(IQ1)	AK064
CCPR = G(IQ2,IQ2)	AK065
DO 176 I=1,IQ1	AK066
176 CCPR = CCPR - G(IQ2,I)*X(I)	AK067
LOGV = .TRUE.	AK068
GO TO 43	AK069
	AK070

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C   SINGULAR MATRIX
774 IF (.NOT. CONVG) GO TO 871
    WRITE (6,172)
172 FORMAT (9H0 (EQLBRM),5X,26HDERIVATIVE MATRIX SINGULAR)
    GO TO 1171
871 WRITE (6,74)
    74 FORMAT (9H0 (EQLBRM),5X,15HSINGULAR MATPIX)
    IF (ISING) GO TO 873
    ISING = .TRUE.
    DO 970 I=1,NS
    IF (EN(I) .NE. 0.) GO TO 970
    EN(I) = SMALNO
    ENLN(I) = SMNOL
970 CONTINUE
    WRITE (6,776)
176 FORMAT (9H0 (EQLBRM),5X,7HRESTART)
    GO TO 43

85 ITNUMB = ITNUMB - 1
C   OBTAIN CORRECTIONS TO THE ESTIMATES
    IF (TP) X(IQ2) = 0.
    DLNT = X(IQ2)
    SUM = X(IQ1)
    DO 101 I=1,NS
    DELN(I) = HRT(I)*DLNT - HPT(I) + (SP(I) - ENLN(I) - TM) + SUM
    DO 99 L=1,NLM
99 DELN(I) = DELN(I) + A(L,I)*X(L)
101 CONTINUE
    AMBDA = 1.
    AMBDA1 = 1.
    SUM = DABS(X(IQ1))
    IF (ABS(DLNT) .GT. SUM) SUM = ABS(DLNT)
    DO 917 I=1,NS
    IF (EN(I) .GT. 0. .AND. DELN(I) .GT. SUM) SUM = DELN(I)
    IF (EN(I) .NE. 0. .OR. DELN(I) .LE. 0.) GO TO 917
    SUM1 = (-9.212 - ENLN(I) + ENNL)/(DELN(I) - X(IQ1))
    SUM1 = ABS(SUM1)
    IF (SUM1 .LT. AMBDA1) AMBDA1 = SUM1
917 CONTINUE
    IF (SUM .GT. 2.) AMBDA = 2./SUM
    IF (AMBDA1 .LT. AMBDA) AMBDA = AMBDA1

C   APPLY CORRECTIONS TO ESTIMATES
    SUM = 0.
    DO 113 I=1,NS
    ENLN(I) = ENLN(I) + AMBDA*DELN(I)
    EN(I) = 0.
    IF ((ENLN(I) - ENNL + SIZE) .LE. 0.) GO TO 113
    EN(I) = EXP(ENLN(I))
    SUM = SUM + EN(I)
113 CONTINUE
    SUMN = SUM
    IF (TP) GO TO 115
    TLN = TLN + AMBDA*DLNT
    TT = EXP(TLN)
    CALL THRM (TT,1.)
    CPSUM = 0.
    DO 3 I=1,NS
    3 CPSUM = CPSUM + CPR(I)*EN(I)
115 ENNL = ENNL + AMBDA*X(IQ1)
    ENN = EXP(ENNL)
    TM = ALOG(PP/ENN)

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AK071
 AK072
 AK073
 AK074
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 AK132
 AK133

C	TEST FOR CONVERGENCE	AK134
	IF (ITNUMB .EQ. 0) GO TO 13	AK135
	IF (AMBDA .LT. 1.) GO TO 43	AK136
	SUM = (ENN - SUMN)/ENN	AK137
	SUM = DABS(SUM)	AK138
	IF (SUM .GT. 0.5E-05) GO TO 43	AK139
	DO 130 I=1,NS	AK140
	AA = ABS(DELN(I)/SUMN)*EN(I)	AK141
	IF (AA .GT. 0.5E-05) GO TO 43	AK142
	130 CONTINUE	AK143
	13 CONVG = .TRUE.	AK144
	IF (ITNUMB .NF. 0) GO TO 160	AK145
	WRITE (6,973) ITN	AK146
973	FORMAT (9H0(EQLBRM),5X,12,52H ITERATIONS DID NOT SATISFY CONVERGEN	AK147
	*CE REQUIREMENTS)	AK148
	GO TO 873	AK149
160	IF (.NOT. (TP .AND. CONVG)) GO TO 143	AK150
	CALL THRM (TT,1.)	AK151
	CPSUM = 0.	AK152
	DO 4 I=1,NS	AK153
4	CPSUM = CPSUM + CPR(I)*EN(I)	AK154
143	ITNUMB = ITN	AK155
	GO TO 43	AK156
		AK157
		AK158
C	CALCULATE EQUILIBRIUM PROPERTIES	AK159
1171	DLVPT = -1.	AK160
	DLVTP = 1.	AK161
	CCPR = CPSUM	AK162
	GO TO 199	AK163
171	SUM = 0.	AK164
	DO 179 L=1,NLM	AK165
179	SUM = SUM + PROW(L)*X(L)	AK166
	DLVPT = -2. + SUM/ENN + X(IQ1)	AK167
199	GAMMA = -1./(DLVPT + DLVTP**2*ENN/CCPR)	AK168
	WM = 1./ENN	AK169
	DO 872 I=1,NS	AK170
872	EN(I) = EXP(ENLN(I))	AK171
	RETURN	AK172
		AK173
873	WRITE (6,900)	AK174
900	FORMAT (9H0(EQLBRM),5X,34HEQUILIBRIUM CALCULATIONS ABANDONED)	AK175
	NEXT = .TRUE.	AK176
	GO TO 171	AK177
		AK178
		AK179
	END	
\$IEFTC	SOUT DECK	AL001
	SUBROUTINE SPOUT	AL002
C	SPECIAL OUTPUT	AL003
	DOUBLE PRECISION EN,ENLN,DELN	AL004
	DOUBLE PRECISION DLVTP,DLVPT	AL005
		AL006
	LOGICAL FROZ	AL007
		AL008
	REAL MIXMW,M2,MACHI,MACHF,M21,LSUBM	AL009
		AL010
	COMMON/KOUT/DUM1(21),UNITO,DUM2(32),FPS,ST,DEUGO	AL011
	COMMON/COND/DVAR,AREA,MDCT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT	AL012
	COMMON/NECC/RR,MIXMW,M2,GAMMAI,TCPR,R	AL013
	COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)	AL014
		AL015

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COMMON/SPEC/DUM3(6),SPNM(2,27),DUM4(25,62)
COMMON/AFUN/CX3,CX2,CX1,CX0,ITPSZ,ISUPP,ETA,D,VISC,BETA
COMMON/MISC/TF,PF,CPR0,HPO,ENN,DUM5(32)
COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)
COMMON/POINTS/DLVTP,DLVET,GAMMAF,WM

ENTRY ECOUT
C EQUILIBRIUM COMBUSTION OUTPUT
WRITE(6,101)
101 FORMAT (1H1,50X,30H** EQUILIBRIUM COMBUSTION **)
VI = 0.
GO TO 2

ENTRY ESOUT
C EQUILIBRIUM SHOCK OUTPUT
WRITE(6,102)
102 FORMAT (1H1,47X,37H** EQUILIBRIUM SHOCK CALCULATION **)

VI= V
2 PI= P
RHOI= RHO
TI= T
P21= PF/PI
T21 = TF/TI
RHO21 = P21/T21*WM/MIXMW
FROZ = .FALSE.
GO TO 3

ENTRY FSOUT
C FROZEN SHOCK OUTPUT
WRITE(6,103)
103 FORMAT (1H1,49X,32H** FROZEN SHOCK CALCULATION **)
PI=P
VI= V
RHOI= RHO
TI=T
P21= PF/PI
T21 = TF/TI
RHO21= P21/T21
P= PF
V= VI/RHO21
RHO= RHOI*RHO21
T= TI*T21
GAMMAF = TCPR/(TCPR - 1./MIXMW)
FROZ = .TRUE.

3 CALL THRM (TI,1.)
PMLOG = ALOG(PI*MIXMW)
S=0.
DO 4 I=1,LS
IF (SIGMA(I) .EQ. 0.) GO TO 4
S = S + SIGMA(I)*(SR(I) - ALOG(SIGMA(I)) - PMLOG)
4 CONTINUE
S = S*1.987165
MACHI= SQRT(M2)

VF = VI/RHO21
RHOV= RHOI*RHO21
CALL THRM (TF,1.)
PMLOG = ALOG(PF*WM)
SF= 0.
DO 5 I=1,LS
IF (EN(I) .EQ. 0.) GO TO 5
SF = SF + FN(I)*(SR(I) - ALOG(EN(I)) - PMLOG)

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NOT REPRODUCIBLE

AL016
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5	CONTINUE	AL080
	SF = SF*1.987165	AL081
	MACHF= SQRT(VF/R*VF/TF*WM/GAMMAF)	AL082
		AL083
	S21= SF/S	AL084
	G21= GAMMAF/GAMMAI	AL085
		AL086
	IF (VI .EQ. 0.) GO TO 205	AL087
	SVI= VI/MACHI	AL088
	SVF= VF/MACHF	AL089
	V21= VF/VI	AL090
	M21= MACHF/MACHI	AL091
	SV21= SVF/SVI	AL092
	GO TO 305	AL093
		AL094
205	MACHI = 0.	AL095
	SVI = 0.	AL096
	SVF = 0.	AL097
	V21 = 0.	AL098
	M21 = 0.	AL099
	SV21 = 0.	AL100
		AL101
305	IF (.NOT. FROZ .OR. ITPSZ .NE. 4) GO TO 405	AL102
C	CALCULATE L(M) FOR KINETIC AREA FUNCTION	AL103
	PST = 1.	AL104
	ROSVST = (GAMMAI/SVI)*1.01325E+06	AL105
	LSUBM = (1./PF)*(RHO21/(RHO21-1.))*(ROSVST/(PST*VISC)*MACHI)**((1.	AL106
	-ETA)/ETA)(D*PI/(4.*BETA))** (1./ETA)	AL107
		AL108
405	WRITE (6,104)	AL109
104	FORMAT (/41X,13HINITIAL STATE,17X,11HFINAL STATE,17X,19HFINAL/INIT	AL110
	*IAL RATIO//)	AL111
		AL112
	IF(UNITO .NE. FPS) GO TO 6	AL113
C	CONVERT FROM INTERNAL (CGS) UNITS TO FPS UNITS	AL114
	PI= PI*2116.2	AL115
	PF= PF*2116.2	AL116
	VI= VI/30.48	AL117
	VF= VF/30.48	AL118
	RHOI= RHOI*62.43	AL119
	RHOF= RHOF*62.43	AL120
	TI= TI*1.8	AL121
	TF= TF*1.8	AL122
	SVI= SVI/30.48	AL123
	SVF= SVF/30.48	AL124
	WRITE(6,105) PI,PF,P21,VI,VF,V21,RHOI,RHOF,RHO21,TI,TF,T21,S,SF,	AL125
	* S21,MACHI,MACHF,M21,GAMMAI,GAMMAF,G21,SVI,SVF,SV21	AL126
105	FORMAT (10X,8HPRESSURE,1PE35.5,E29.5,E32.5/11X,10H(LB/FT**2)/10X,	AL127
	* 8HVELOCITY,E35.5,E29.5,E32.5/11X,8H(FT/SEC)/10X,7HDENSITY,E36.5,	AL128
	* E29.5,E32.5/11X,10H(LB/FT**3)/10X,11HTEMPERATURE,E32.5,E29.5,	AL129
	* E32.5/11X,7H(DEG R)/10X,7HENTROPY,E36.5,E29.5,E32.5/11X,14H(BTU/L	AL130
	*E/DEG R)/10X,11HMACH NUMBER,E32.5,E29.5,E32.5//10X,5HGAMMA,E38.5,	AL131
	* E29.5,E32.5//10X,14HSONIC VELOCITY,E29.5,E29.5,E32.5/11X,8H(FT/SE	AL132
	*C))	AL133
	GO TO 8	AL134
		AL135
6	IF (UNITO .NE. SI) GO TO 7	AL136
C	CONVERT FROM INTERNAL (CGS) UNITS TO SI UNITS	AL137
	PI= PI*1.01325E+05	AL138
	PF= PF*1.01325E+05	AL139
	VI= VI*0.01	AL140


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VF= VF*0.01
RHOI= RHOI*1000.
RHOF= RHOF*1000.
S= S*4184.0
SF= SF*4184.0
SVI= SVI*0.01
SVF= SVF*0.01
WRITE(6,106) PI,PF,P21,VI,VF,V21,RHOI,RHOF,RHO21,TI,TF,T21,S,SF,
* S21,MACHI,MACHF,M21,GAMMAI,GAMMAF,G21,SVI,SVF,SV21
106 FORMAT (10X,8HPRESSURE,1PE35.5,E29.5,E32.5/11X,8H(N/M**2)/10X,8HVE
*LOCITY,E35.5,E29.5,E32.5/11X,7H(M/SEC)/10X,7HDENSITY,E36.5,E29.5,
* E32.5/11X,9H(KG/M**2)/10X,11HTEMPERATURE,E32.5,E29.5,E32.5/11X,
* 7H(DEG K)/10X,7HENTROPY,E36.5,E29.5,E32.5/11X,16H(JOULE/KG/DEG K)
*/10X,11HMACH NUMBER,E32.5,E29.5,E32.5//10X,5HGAMMA,E38.5,E29.5,
* E32.5//10X,14HSONIC VELOCITY,E29.5,E29.5,E32.5/11X,7H(M/SEC))
GO TO 8
C PRINT OUTPUT IN INTERNAL (CGS) UNITS
7 WRITE(6,107) PI,PF,P21,VI,VF,V21,RHOI,RHOF,RHO21,TI,TF,T21,S,SF,
* S21,MACHI,MACHF,M21,GAMMAI,GAMMAF,G21,SVI,SVF,SV21
107 FORMAT (10X,8HPRESSURE,F35.4,F28.4,F32.4/11X,5H(ATM)/10X,8HVELOCIT
*Y,F33.2,F28.2,F34.4/11X,8H(CM/SEC)/10X,7HDENSITY,1PE36.5,E28.5,
* OPF32.4/11X,10H(GM/CM**3)/10X,11HTEMPERATURE,F30.2,F28.2,F34.4/
* 11X,7H(DEG K)/10X,7HENTROPY,F36.4,F28.4,F32.4/11X,14H(CAL/GM/DEG
*K)/10X,11HMACH NUMBER,F32.4,F28.4,F32.4//10X,5HGAMMA,F38.4,F28.4,
* F32.4//10X,14HSONIC VELOCITY,F27.2,F28.2,F34.4/11X,8H(CM/SEC))
8 WRITE(6,108)
108 FORMAT (/67X,7HSPECIES,5X,13HMOLE FRACTION)
DO 9 I=1,LS
EN(I) = EN(I)*WM
WRITE(6,109) (SPNM(K,I),K=1,2),EN(I)
109 FORMAT (68X,2A4,3X,1PE12.5)
9 CONTINUE
WRITE(6,110) WM,DLVTP,DLVPT
110 FORMAT (/10X,24HMIXTURE MOLECULAR WEIGHT,36X,F12.5//10X,22HD(LOG V
*OLUME)/D(LOG T),F49.4/14X,13HAT CONSTANT P//10X,22HD(LOG VOLUME)/D
*(LOG P),F49.4/14X,13HAT CONSTANT T)
RETURN
END
$IEFTC OUTPP DECK
SUBROUTINE OUTP
C OUTPUT CAN BE GIVEN IN (1) INTERNAL (CGS) UNITS, (2) FPS UNITS
C (3) SI UNITS
LOGICAL ALLM1,CONC,DBUGO,EXCHR,NEXT,RHOCON,TCON
REAL MDOT,IVAR,N,M,MW,MIXMW,M2,MACH,LSUBM
DIMENSION SPNM(2,27),PRC(25),PRX(30),XXH(30),ESP(2,25)
COMMON/OPTS/VERSI,TIMEV,VERSA,ARFAV,ELIM,TCON,PHOCON,IPRCOD
COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT
COMMON/SINT/HMIN,HINT,HN,HNP1,HMAX,NH,AVH,EMAX,ERRN,JCV,KOUNT,ERRP
COMMON/KOUT/TITLE(20),UNITI,UNITO,CONC,EXCHR,DELH(30),FPS,SI,DBUGO
COMMON/REAC/LSR(4,30),XX(30),RATE(30),LKEQ(30),DLKEQ(30),MM(30),LP
COMMON/RRAT/A(30),N(30),EACT(30),B(30),M(25,30),ALLM1
COMMON/AFUN/CN(4),ITPSZ,LSURM,ETA,D,VISC,BETAL
COMMON/SPEC/SNAM(2,30),MW(25),W(25),STOIC(25,30),OMEGA(25,30)

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COMMON/XVSA/XTB(40),ATB(40),NTB,XU,AU(2),CX(4)	AM020
COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R	AM021
COMMON/PQRE/PK(28),QK(28),RK(28),E(28)	AM022
COMMON/DERN/F(28),ALPHA(28),BETA(28,28)	AM023
COMMON/SKIP/NEGL(25),I1,I2,IT	AM024
COMMON/GHSC/GRT(25),HRT(25),SR(25),CPF(25),DCPR(25)	AM025
COMMON/SABS/S1,AA,BB,S2,DA,D2A,DTERM	AM026
	AM027
EQUIVALENCE (SPNM,SNAM(1,4)),(BLANK,SPNM(1,27))	AM028
EQUIVALENCE (PRX(1),XXH(1))	AM029
	AM030
ENTRY OUT1	AM031
	AM032
C ** TITLE PAGE	AM033
IF (VERSI .EQ. TIMEV) GO TO 98	AM034
I = 2	AM035
GO TO 99	AM036
98 I = 4	AM037
99 IF (VERSA .EQ. AREAV) I = I - 1	AM038
GO TO (100,200,300,400),I	AM039
100 WRITE (6,101)	AM040
101 FORMAT (1H1,14X,21HDISTANCE-AREA VERSION)	AM041
GO TO 3	AM042
200 WRITE (6,201)	AM043
201 FORMAT (1H1,12X,25HDISTANCE-PRESSURE VERSION)	AM044
GO TO 3	AM045
300 WRITE (6,301)	AM046
301 FORMAT (1H1,16X,17HTIME-AREA VERSION)	AM047
GO TO 3	AM048
400 WRITE (6,401)	AM049
401 FORMAT (1H1,14X,21HTIME-PRESSURE VERSION)	AM050
3 WRITE (6,102) (TITLE(I),I=1,20)	AM051
102 FORMAT (1H+,49X,33HGENERAL CHEMICAL KINETICS PROGRAM,11X,26HNASA L	AM052
*EWIS RESEARCH CENTER///26X,20A4///9X,8HREACTION,31X,8HREACTION,	AM053
* 38X,23HREACTION RATE VARIABLES/10X,6HNUMBER,74X,1HA,16X,1HN,9X,	AM054
* 10HACTIVATION/119X,6HENERGY)	AM055
	AM056
C PRINT REACTION INFORMATION	AM057
DO 6 J=1,LR	AM058
N1 = LSR(1,J)	AM059
N2 = LSR(2,J)	AM060
N3 = LSR(3,J)	AM061
N4 = LSR(4,J)	AM062
WRITE (6,103) J, (SPNM(I,N2),I=1,2), (SPNM(I,N3),I=1,2), A(J), N(J),	AM063
* EACT(J)	AM064
103 FORMAT (12X,I2,27X,2A4,2X,1H=,2X,2A4,23X,1PE12.5,5X,0PF10.4,5X,	AM065
* F10.2)	AM066
IF (N1 .GT. 0) GO TO 5	AM067
IF (N1 .LT. 0) GO TO 4	AM068
N1 = 26	AM069
GO TO 205	AM070
4 WRITE (6,105) (SPNM(I,N4),I=1,2)	AM071
105 FORMAT (1H+,63X,1H+,2X,2A4)	AM072
GO TO 6	AM073
5 IF (N4 .GT. 0) GO TO 205	AM074
IF (N4 .LT. 0) GO TO 204	AM075
N4 = 26	AM076
GO TO 205	AM077
204 WRITE (6,1105) (SPNM(I,N1),I=1,2)	AM078
1105 FORMAT (1H+,27X,2A4,2X,1H+)	AM079
GO TO 6	AM080

205	WRITE (6,104) (SPNM(I,N1),I=1,2), (SPNM(I,N4),I=1,2)	AM081
104	FORMAT (1H+,27X,2A4,2X,1H+,25X,1H+,2X,2A4)	AM082
C	CONVERT ACTIVATION ENERGY TO B-FACTOR	AM083
6	B(J) = EACT(J)/1.987165	AM084
	IF (.NOT. ALLM1) GO TO 7	AM085
	WRITE (6,106)	AM086
106	FORMAT (///51X,29HALL THIRD BODY RATIOS ARE 1.0)	AM087
	GO TO 13	AM088
		AM089
		AM090
7	WRITE (6,107)	AM091
107	FORMAT (///41X,50HALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWI	AM092
	*NG//)	AM093
	K = 0	AM094
	DO 12 I=1,LS	AM095
	DO 12 J=1,LR	AM096
	IF (M(I,J) .EQ. 1.) GO TO 12	AM097
	K = K + 1	AM098
	IF (K .EQ. 5) K = 1	AM099
	GO TO (8,9,10,11),K	AM100
8	WRITE (6,108) (SPNM(K,I),K=1,2),J,M(I,J)	AM101
108	FORMAT (5X,2HM(,2A4,1H,,I2,3H) =,F10.5)	AM102
	GO TO 12	AM103
9	WRITE (6,109) (SPNM(K,I),K=1,2),J,M(I,J)	AM104
109	FORMAT (1H+,36X,2HM(,2A4,1H,,I2,3H) =,F10.5)	AM105
	GO TO 12	AM106
10	WRITE (6,110) (SPNM(K,I),K=1,2),J,M(I,J)	AM107
110	FORMAT (1H+,68X,2HM(,2A4,1H,,I2,3H) =,F10.5)	AM108
	GO TO 12	AM109
11	WRITE (6,111) (SPNM(K,I),K=1,2),J,M(I,J)	AM110
111	FORMAT (1H+,100X,2HM(,2A4,1H,,I2,3H) =,F10.5)	AM111
12	CONTINUE	AM112
		AM113
		AM114
13	IF (VERSI .EQ. TIMEV) GO TO 14	AM115
	WRITE (6,112) HMIN,HMAX,HINT,EMAX	AM116
112	FORMAT (///56X,20HINTEGRATION CONTROLS//15X,17HMINIMUM STEP SIZE,	AM117
	* E14.5,3H CM,33X,17HMAXIMUM STEP SIZE,E14.5,3H CM//15X,17HINITIAL	AM118
	*STEP SIZE,E14.5,3H CM,33X,22HMAXIMUM RELATIVE ERROR,F10.5)	AM119
	GO TO 15	AM120
14	WRITE (6,113) HMIN,HMAX,HINT,EMAX	AM121
113	FORMAT (///56X,20HINTEGRATION CONTROLS//15X,17HMINIMUM STEP SIZE,	AM122
	* E14.5,4H SEC,32X,17HMAXIMUM STEP SIZE,E14.5,4H SEC//15X,17HINITIA	AM123
	*L STEP SIZE,E14.5,4H SEC,32X,22HMAXIMUM RELATIVE ERROR,F10.5)	AM124
		AM125
C **	SECOND PAGE	AM126
15	WRITE (6,114)	AM127
114	FORMAT (1H1,50X,31H** ASSIGNED VARIABLE PROFILE **//)	AM128
	GO TO (16,18,19,20),ITPSZ	AM129
		AM130
16	GO TO (116,216,316,416),IPRCOD	AM131
C	ASSIGNED VARIABLE TABLE	AM132
116	WRITE (6,117) XU,AU	AM133
117	FORMAT (34X,64HTHE AREA IS CALCULATED BY INTERPOLATION FROM THE FO	AM134
	*LLOWING TABLE//36X,7HSTATION,10X,17HAXIAL DISTANCE (,A2,1H),10X,	AM135
	* 7HAREA (,A4,A1,1H))	AM136
	GO TO 516	AM137
216	WRITE (6,217) XU,AU	AM138
217	FORMAT (32X,68HTHE PRESSURE IS CALCULATED BY INTERPOLATION FROM TH	AM139
	*E FOLLOWING TABLE//36X,7HSTATION,10X,17HAXIAL DISTANCE (,A2,1H),	AM140
	* 9X,11HPRESSURE (,2A4,1H))	AM141
	GO TO 516	AM142

316	WRITE (6,317) AU	AM143
317	FORMAT (34X,64H)THE AREA IS CALCULATED BY INTERPOLATION FROM THE FO	AM144
	*LLOWING TABLE//36X,7HSTATION,14X,11HTIME (SEC),16X,7HAREA (.A4,	AM145
	* A1,1H))	AM146
	GO TO 516	AM147
416	WRITE (6,417) AU	AM148
417	FORMAT (32X,68H)THE PRESSURE IS CALCULATED BY INTERPOLATION FROM TH	AM149
	*E FOLLOWING TABLE//36X,7HSTATION,14X,11HTIME (SEC),15X,11HPRESSUR	AM150
	*E (.2A4,1H))	AM151
516	DO 17 I=1,NTB	AM152
17	WRITE (6,616) I,XTB(I),ATB(I)	AM153
616	FORMAT (38X,I2,14X,1PE12.5,15X,E12.5)	AM154
	GO TO 21	AM155
		AM156
	18 GO TO (218,318,418,518),IPRCOD	AM157
C	ASSIGNED VARIABLE POLYNOMIAL	AM158
218	WRITE (6,219) AU,CX	AM159
219	FORMAT (40X,52H)THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIA	AM160
	*L//23X,6HAREA (.A4,A1,5H) = (.1PE12.5,9H)X**3 + (.E12.5,9H)X**2 +	AM161
	* (.E12.5,6H)X + (.E12.5,1H))	AM162
	GO TO 21	AM163
318	WRITE (6,319) AU,CX	AM164
319	FORMAT (38X,56H)THE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYN	AM165
	*OMIAL//20X,10HPRESSURE (.2A4,5H) = (.1PE12.5,9H)X**3 + (.E12.5,9H)	AM166
	*X**2 + (.E12.5,6H)X + (.E12.5,1H))	AM167
	GO TO 21	AM168
418	WRITE (6,419) AU,CX	AM169
419	FORMAT (40X,52H)THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIA	AM170
	*L//23X,6HAREA (.A4,A1,5H) = (.1PE12.5,9H)T**3 + (.E12.5,9H)T**2 +	AM171
	* (.E12.5,6H)T + (.E12.5,1H))	AM172
	GO TO 21	AM173
518	WRITE (6,519) AU,CX	AM174
519	FORMAT (38X,56H)THE PRESSURE IS CALCULATED FROM THE FOLLOWING POLYN	AM175
	*OMIAL//20X,10HPRESSURE (.2A4,5H) = (.1PE12.5,9H)T**3 + (.E12.5,9H)	AM176
	*T**2 + (.E12.5,6H)T + (.E12.5,1H))	AM177
	GO TO 21	AM178
		AM179
C	SPECIAL AREA FUNCTION	AM180
19	WRITE (6,118) LSUBM,ETA	AM181
118	FORMAT (41X,50H)THE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION/	AM182
	* /46X,16H1/AREA = 1 - (X/,F10.3,4H)**(.F10.5,1H))	AM183
	IF (ITPSZ .EQ. 4) WRITE (6,1118) D,VISC,BETAL	AM184
1118	FORMAT (/6X,20H)HYDRAULIC DIAMETER =,F8.4,3H CM,7X,23H)VISCOISITY COE	AM185
	*FFICIENT =,E12.4,10H GM/CM-SEC,7X,6HBETA =,F7.4)	AM186
	GO TO 21	AM187
		AM188
C	ZERO VELOCITY - ASSIGNED VARIABLE NOT REQUIRED	AM189
20	WRITE (6,119)	AM190
119	FORMAT (36X,60H)THIS IS A V=0 PROBLPM - AN ASSIGNED VARIABLE IS NOT	AM191
	* REQUIRED)	AM192
		AM193
C	NEGLECTED SPECIES	AM194
21	IF (I1 .NE. 0) GO TO 22	AM195
	WRITE (6,120)	AM196
120	FORMAT (///31X,70H)NO SPECIES WILL BE PERMANENTLY NEGLECTED FROM AL	AM197
	*L ERROR CONSIDERATIONS)	AM198
	GO TO 228	AM199
22	WRITE (6,121)	AM200
121	FORMAT (///31X,69H)THE FOLLOWING SPECIES WILL BE NEGLFCTED FROM ALL	AM201
	* ERROR CONSIDERATIONS//)	AM202
	K = 0	AM203
	DO 28 II=1,I1	AM204

NOT REPRODUCIBLE

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I = NEGL(II)
K = K + 1
IF (K .EQ. 6) K = 1
GO TO (23,24,25,26,27),K
23 WRITE (6,122) (SPNM(J,I),J=1,2)
122 FORMAT (61X,2A4)
GO TO 28
24 WRITE (6,123) (SPNM(J,I),J=1,2)
123 FORMAT (1H+,76X,2A4)
GO TO 28
25 WRITE (6,124) (SPNM(J,I),J=1,2)
124 FORMAT (1H+,44X,2A4)
GO TO 28
26 WRITE (6,125) (SPNM(J,I),J=1,2)
125 FORMAT (1H+,92X,2A4)
GO TO 28
27 WRITE (6,126) (SPNM(J,I),J=1,2)
126 FORMAT (1H+,28X,2A4)
28 CONTINUE

228 IF (RHOCON) WRITE (6,1126)
1126 FORMAT (///38X,56HTHE VOLUME (DENSITY) WILL BE HELD CONSTANT FOR T
*HIS CASE)
IF (TCON) WRITE (6,2126)
2126 FORMAT (///40X,51HTHE TEMPERATURE WILL BE HELD CONSTANT FOR THIS C
*ASE)
RETURN

ENTRY OUT2

C INITIAL CONDITIONS
WRITE (6,127)
127 FORMAT (1H1,52X,26H** INITIAL CONDITIONS **//)
GO TO 29

ENTRY OUT3

C GENERAL OUTPUT
WRITE (6,128)
128 FORMAT (1H1)

29 MACH = SQRT(M2)
MAX = MAX0(LS,LR)

TENT = 0.
CSUM = 0.
PMLOG = ALOG(P*MIXMW)
C TOTAL ENTROPY AND MASS FRACTION SUM
DO 30 I=1,LS
IF (SIGMA(I) .EQ. 0.) GO TO 30
TENT = TENT + SIGMA(I)*(SR(I) - ALOG(SIGMA(I)) - PMLOG)
30 CSUM = CSUM + SIGMA(I)*MW(I)
TENT = TENT*1.987165

TXXH = 0.
C ENERGY EXCHANGE RATES
DO 31 J=1,LR
XXH(J) = XX(J)*DELH(J)
31 TXXH = TXXH + XXH(J)

IF (VERSI .EQ. TIMEV) GO TO 32
TIME = DVAR
X = IVAR
GO TO 33

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AM205
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 AM268

32	TIME = IVAR	AM269
	X = DVAR	AM270
33	IF (UNITO .NE. FPS) GO TO 48	AM271
		AM272
		AM273
C	CONVERT FROM INTERNAL (CGS) UNITS TO FPS UNITS	AM274
	X = X/30.48	AM275
	AREAA = AREA/929.0304	AM276
	DOTM = MDOT/453.59237	AM277
	PP = P*2116.2	AM278
	VV = V/30.48	AM279
	RHOO = RHO*62.43	AM280
	TT = T*1.8	AM281
		AM282
	WRITE (6,129) TIME,AREAA,X,PP,NH,VV,AVH,RHOO,(SNAM(I,JCV),I=1,2),	AM283
	* TT,DOTM,TENT,ERRN,MACH,KOUNT,GAMMA	AM284
129	FORMAT (16X,4HTIME,1PE14.5,5H SEC,14X,4HAREA,E14.5,7H SQ FT,	AM285
	* 14X,14HAXIAL POSITION,E14.5,4H FT///20X,15HFLOW PROPERTIES,45X,	AM286
	* 22HINTEGRATION INDICATORS//22X,8HPRESSURE,E22.5,30X,21HSTEPS FR	AM287
	*OM LAST PRINT,9X,14/23X,10H (LB/FT**2)/22X,8HVELOCITY,E22.5,30X,	AM288
	* 17HAVERAGE STEP SIZE,0PE24.5/23X,8H (FT/SEC)/22X,7HDENSITY,1PE23.5	AM289
	*,30X,20HCONTROLLING VARIABLE,11X,2A4/23X,10H (LB/FT**3)/22X,11HTEMP	AM290
	*ERATURE,E19.5/23X,7H (DEG R)/22X,14HMASS FLOW RATE,E16.5/23X,8H (LB/	AM291
	*SEC)/22X,7HENTROPY,E23.5,30X,14HRELATIVE ERROR,0PE27.5/23X,14H (BTU	AM292
	* /LB/DEG R)/22X,11HMACH NUMBER,1PE19.5,30X,20HPREDICTOR ITERATIONS,	AM293
	* 11X,13//22X,5HGAMMA,E25.5)	AM294
		AM295
	IF (I2 .EQ. 0) GO TO 34	AM296
	IS = I1 + 1	AM297
	DO 233 K=IS,IT	AM298
	KK = NEGL(K)	AM299
	ESP(1,K) = SPNM(1,KK)	AM300
233	ESP(2,K) = SPNM(2,KK)	AM301
	WRITE (6,130) ((ESP(I,K),I=1,2),K=IS,IT)	AM302
130	FORMAT (1H+,81X,18HELIMINATED SPECIES,13X,2A4,2X,2A4/(113X,2A4,2X,	AM303
	* 2A4))	AM304
		AM305
34	WRITE (6,131)	AM306
131	FORMAT (//56X,19HCHEMICAL PROPERTIES//)	AM307
		AM308
	CONV = 0.02883	AM309
	IF (CONC .OR. EXCHR) GO TO 36	AM310
		AM311
C	PRINT MASS FRACTIONS AND REACTION CONVERSION RATES	AM312
	WRITE (6,132)	AM313
132	FORMAT (1X,7HSPECIES,4X,13HMASS FRACTION,3X,13HMOLE FRACTION,3X,	AM314
	* 27HNET SPECIES PRODUCTION RATE,5X,8HREACTION,3X,28HNET REACTION C	AM315
	*ONVERSION RATE,3X,13HRAE CONSTANT)	AM316
	WRITE (6,133)	AM317
133	FORMAT (50X,16H (MOLE/FT**3/SEC),11X,6HNUMBER,7X,22H (MOLE-FT**3/LP	AM318
	**2/SEC),7X,11H (CGS UNITS))	AM319
	DO 35 J=1,LP	AM320
35	PRX(J) = XX(J)	AM321
	CONV = 1./62.43	AM322
	GO TO 37	AM323
		AM324
36	IF (CONC .OR. (.NOT. EXCHR)) GO TO 39	AM325
		AM326
C	PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES	AM327
	WRITE (6,134)	AM328

134	FORMAT (1X,7HSPECIES,4X,13HMASS FRACTION,3X,13HMOLE FRACTION,3X,	AM329
	* 27HNET SPECIES PRODUCTION RATE,5X,8HREACTION,5X,24HNET ENERGY EXC	AM330
	*HANGE RATE,5X,13HRAE CONSTANT)	AM331
	WRITE (6,135)	AM332
135	FORMAT (50X,16H (MOLE/FT**3/SEC),11X,6HNUMBER,8X,21H (BTU-FT**3/LB**	AM333
	*2/SEC),7X,11H (CGS UNITS))	AM334
		AM335
C	COMPUTE MASS FRACTIONS	AM336
37	DO 38 I=1,LS	AM337
38	PRC(I) = SIGMA(I)*MW(I)	AM338
	GO TO 44	AM339
		AM340
39	IF ((.NOT. CONC) .OR. EXCHR) GO TO 41	AM341
		AM342
C	PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES	AM343
	WRITE (6,136)	AM344
136	FORMAT (1X,7HSPECIES,4X,13HCONCENTRATION,3X,13HMOLE FRACTION,3X,	AM345
	* 27HNET SPECIES PRODUCTION RATE,5X,8HREACTION,3X,28HNFT REACTION C	AM346
	*ONVERSION RATE,3X,13HRAE CONSTANT)	AM347
	WRITE (6,137)	AM348
137	FORMAT (12X,13H (MOLES/FT**3),25X,16H (MOLE/FT**3/SEC),11X,6HNUMBER,	AM349
	* 7X,22H (MOLE-FT**3/LB**2/SEC),7X,11H (CGS UNITS))	AM350
	DO 40 J=1,LR	AM351
40	PRX(J) = XX(J)	AM352
	CONV = 1./62.43	AM353
	GO TO 42	AM354
		AM355
C	PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES	AM356
41	WRITE (6,138)	AM357
138	FORMAT (1X,7HSPECIES,4X,13HCONCENTRATION,3X,13HMOLE FRACTION,3X,	AM358
	* 27HNET SPECIES PRODUCTION RATE,5X,8HREACTION,5X,24HNET ENERGY EXC	AM359
	*HANGE RATE,5X,13HRAE CONSTANT)	AM360
	WRITE (6,139)	AM361
139	FORMAT (12X,13H (MOLES/FT**3),25X,16H (MOLE/FT**3/SEC),11X,6HNUMBER,	AM362
	* 8X,21H (BTU-FT**3/LB**2/SEC),7X,11H (CGS UNITS))	AM363
		AM364
		AM365
C	COMPUTE MOLAR CONCENTRATIONS	AM366
42	DO 43 I=1,LS	AM367
43	PRC(I) = SIGMA(I)*RHOO	AM368
		AM369
44	DO 47 IJ=1,MAX	AM370
	IF (IJ .GT. LS .OR. IJ .GT. LR) GO TO 45	AM371
	FMOL = SIGMA(IJ)*MIXMW	AM372
	WW = W(IJ)*62.43	AM373
	XXX = PRX(IJ)*CONV	AM374
	WRITE (6,140) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,WW,IJ,XXX,RATE(IJ)	AM375
140	FORMAT (2X,2A4,2X,1PE12.5,4X,E12.5,11X,E12.5,16X,I2,14X,E12.5,11X,	AM376
	* E12.5)	AM377
	GO TO 47	AM378
45	IF (IJ .GT. LS) GO TO 46	AM379
	FMOL = SIGMA(IJ)*MIXMW	AM380
	WW = W(IJ)*62.43	AM381
	WRITE (6,141) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,WW	AM382
141	FORMAT (2X,2A4,2X,1PE12.5,4X,E12.5,11X,E12.5)	AM383
	GO TO 47	AM384
46	XXX = PRX(IJ)*CONV	AM385
	WRITE (6,142) IJ,XXX,RATE(IJ)	AM386
142	FORMAT (79X,I2,14X,1PE12.5,11X,E12.5)	AM387
47	CONTINUE	AM388
	TXXH = TXXH*0.02883	AM389
	WRITE (6,143) MIXMW,TXXH,CSUM	

143	FORMAT (/4X,24HMIXTURE MOLECULAR WEIGHT,F13.5,5X,26HTOTAL ENERGY	AM390
	*EXCHANGE RATE,1PE15.5,7X,17HMASS FRACTION SUM,0PF14.8)	AM391
	WRITE (6,144)	AM392
144	FORMAT (49X,21H(BTU-FT**3/LB**2/SEC))	AM393
	GO TO 78	AM394
		AM395
48	IF (UNITO .NE. SI) GO TO 63	AM396
		AM397
C	CONVERT FROM INTERNAL (CGS) UNITS TO SI UNITS	AM398
	X = X*.01	AM399
	AREAA = AREA*.0001	AM400
	DOTM = MDOT*0.001	AM401
	PP = P*1.01325E+05	AM402
	VV = V*.C1	AM403
	RHOO = RHO*1000.	AM404
	TENT = TENT*4184.0	AM405
		AM406
	WRITE (6,145) TIME,AREAA,X,PP,NH,VV,AVH,RHOO,(SNAM(I,JCV),I=1,2),	AM407
	* T,DOTM,TENT,ERRN,MACH,KOUNT,GAMMA	AM408
145	FORMAT (16X,4HTIME,1PE14.5,5H SEC,14X,4HAREA,E14.5,7H SQ M,	AM409
	* 14X,14HAXIAL POSITION,E14.5,4H M ///20X,15HFLOW PROPERTIES,45X,	AM410
	* 22HINTEGRATION INDICATORS//22X,8HPRESSURE,E22.5,30X,21HSTEPS FR	AM411
	*OM LAST PRINT,9X,I4/23X,8H(N/M**2)/22X,8HVELOCITY,E22.5,30X,17HAVE	AM412
	*RAGE STEP SIZE,0PE24.5/23X,7H(M/SEC)/22X,7HDENSITY,1PE23.5,30X,	AM413
	* 20HCONTROLLING VARIABLE,11X,2A4/23X,9H(KG/M**3)/22X,11HTEMPERATUR	AM414
	*E,E19.5/23X,7H(DEG K)/22X,14HMASS FLOW RATE,E16.5/23X,8H(KG/SFC)/	AM415
	* 22X,7HENTROPY,E23.5,30X,14HRELATIVE ERROR,0PE27.5/23X,16H(JOULF/K	AM416
	*G/DEG K)/22X,11HMACH NUMBER,1PE19.5,30X,20HPREDICTOR ITERATIONS,	AM417
	* 11X,I3//22X,5HGAMMA,E25.5)	AM418
		AM419
	IF (I2 .EQ. 0) GO TO 49	AM420
	IS = I1 + 1	AM421
	DO 248 K=IS,IT	AM422
	KK = NEGL(K)	AM423
	ESP(1,K) = SPNM(1,KK)	AM424
248	ESP(2,K) = SPNM(2,KK)	AM425
	WRITE (6,130) ((ESP(I,K),I=1,2),K=IS,IT)	AM426
		AM427
49	WRITE (6,131)	AM428
		AM429
	CONV = 4.1840	AM430
	IF (CONC .OR. EXCHR) GO TO 51	AM431
		AM432
C	PRINT MASS FRACTIONS AND REACTION CONVERSION RATES	AM433
	WRITE (6,132)	AM434
	WRITE (6,146)	AM435
146	FORMAT (50X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X,21H(MOLE-M**3/KG**2	AM436
	*/SEC),8X,11H(CGS UNITS))	AM437
	DO 50 J=1,LR	AM438
50	PRX(J) = XX(J)	AM439
	CONV = 0.001	AM440
	GO TO 52	AM441
		AM442
51	IF (CONC .OR. (.NOT. FXCHR)) GO TO 54	AM443
		AM444
C	PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES	AM445
	WRITE (6,134)	AM446
	WRITE (6,147)	AM447
147	FORMAT (50X,15H(MOLE/M**3/SFC),12X,6HNUMBER,7X,22H(JOULF-M**3/KG**	AM448
	*2/SEC),7X,11H(CGS UNITS))	AM449
		AM450

C	COMPUTE MASS FRACTIONS	AM451
	52 DO 53 I=1,LS	AM452
	53 PRC(I) = SIGMA(I)*MW(I)	AM453
	GO TO 59	AM454
		AM455
	54 IF ((.NOT. CONC) .OR. EXCHR) GO TO 56	AM456
		AM457
C	PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES	AM458
	WRITE (6,136)	AM459
	WRITE (6,148)	AM460
	148 FORMAT (12X,12H(MOLES/M**3),26X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X	AM461
	*,21H(MOLE-M**3/KG**2/SEC),8X,11H(CGS UNITS))	AM462
	DO 55 J=1,LR	AM463
	55 PRX(J) = XX(J)	AM464
	CONV = 0.001	AM465
	GO TO 57	AM466
		AM467
C	PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES	AM468
	56 WRITE (6,138)	AM469
	WRITE (6,149)	AM470
	149 FORMAT (12X,12H(MOLES/M**3),26X,15H(MOLE/M**3/SEC),12X,6HNUMBER,7X	AM471
	*,22H(JOULE-M**3/KG**2/SEC),7X,11H(CGS UNITS))	AM472
		AM473
C	COMPUTE MOLAR CONCENTRATIONS	AM474
	57 DO 58 I=1,LS	AM475
	58 PRC(I) = SIGMA(I)*RHOO	AM476
		AM477
	59 DO 62 IJ=1,MAX	AM478
	IF (IJ .GT. LS .OR. IJ .GT. LR) GO TO 60	AM479
	FMOL = SIGMA(IJ)*MIXMW	AM480
	WW = W(IJ)*1000.	AM481
	XXX = PRX(IJ)*CONV	AM482
	WRITE (6,140) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,WW,IJ,XXX,RATE(IJ)	AM483
	GO TO 62	AM484
	60 IF (IJ .GT. LS) GO TO 61	AM485
	FMOL = SIGMA(IJ)*MIXMW	AM486
	WW = W(IJ)*1000.	AM487
	WRITE (6,141) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,WW	AM488
	GO TO 62	AM489
	61 XXX = PRX(IJ)*CONV	AM490
	WRITE (6,142) IJ,XXX,RATE(IJ)	AM491
	62 CONTINUE	AM492
	TXXH = TXXH*4.1840	AM493
	WRITE (6,143) MIXMW,TXXH,CSUM	AM494
	WRITE (6,150)	AM495
	150 FORMAT (48X,22H(JOULE-M**3/KG**2/SFC))	AM496
	GO TO 78	AM497
		AM498
		AM499
C	PRINT OUTPUT IN INTERNAL (CGS) UNITS	AM500
	63 WRITE (6,151) TIME,AREA,X,P,NH,V,AVH,PHO,(SNAM(I,JCV),I=1,2),	AM501
	* T,MDOT,TENT,ERRN,MACH,KCUNT,GAMMA	AM502
	151 FORMAT (16X,4HTIME,1PE14.5,5H SEC,14X,4HAREA,E14.5,7H SQ CM,	AM503
	* 14X,14HAXIAL POSITION,E14.5,4H CM//20X,15HFLOW PROPERTIES,45X,2	AM504
	*2HINTEGRATION INDICATORS//22X,8HPRESSURE,0PF23.5,29X,21HSTEPS FROM	AM505
	* LAST PRINT,9X,I4/23X,5H(ATM)/22X,8HVELOCITY,F20.2,32X,17HAFRAGE	AM506
	*STEP SIZE,E24.5/23X,8H(CM/SEC)/22X,7HDENSITY,1PE23.5,30X,20HCONTRO	AM507
	*LLING VAPIABLE,11X,2A4/23X,10H(GM/CM**3)/22X,11HTFMPERATURE,	AM508
	* 0PF17.2/23X,7H(DEG K)/22X,14HMASS FLOW RATE,1PE16.5/23X,8H(GM/SEC	AM509
	*)/22X,7HENTROPY,0PF23.4,30X,14HRELATIVE ERROR,E27.5/23X,14H(CAL/GM	AM510
	*/DEG K)/22X,11HMACH NUMBER,F19.4,30X,20HPREDICTOR ITERATIONS,11X,	AM511
	* I3//22X,5HGAMMA,F25.4)	AM512

IF (I2 .EQ. 0) GO TO 64	AM513
IS = I1 + 1	AM514
DO 263 K=IS,IT	AM515
KK = NEGL(K)	AM516
ESP(1,K) = SPNM(1,KK)	AM517
263 ESP(2,K) = SPNM(2,KK)	AM518
WRITE (6,130) ((ESP(I,K),I=1,2),K=IS,IT)	AM519
	AM520
64 WRITE (6,131)	AM521
	AM522
IF (CONC .OR. EXCHR) GO TO 66	AM523
	AM524
C PRINT MASS FRACTIONS AND REACTION CONVERSION RATES	AM525
WRITE (6,132)	AM526
WRITE (6,152)	AM527
152 FORMAT (50X,16H(MOLE/CM**3/SEC),11X,6HNUMBER,7X,22H(MOLE-CM**3/GM**2/SEC),7X,11H(CGS UNITS))	AM528
DO 65 J=1,LR	AM529
65 PRX(J) = XX(J)	AM530
GO TO 67	AM531
	AM532
	AM533
66 IF (CONC .OR. (.NOT. EXCHR)) GO TO 69	AM534
	AM535
C PRINT MASS FRACTIONS AND ENERGY EXCHANGE RATES	AM536
WRITE (6,134)	AM537
WRITE (6,153)	AM538
153 FORMAT (50X,16H(MOLE/CM**3/SEC),11X,6HNUMBER,8X,21H(CAL-CM**3/GM**2/SEC),7X,11H(CGS UNITS))	AM539
	AM540
	AM541
C COMPUTE MASS FRACTIONS	AM542
67 DO 68 I=1,LS	AM543
68 PRC(I) = SIGMA(I)*MW(I)	AM544
GO TO 74	AM545
	AM546
69 IF ((.NOT. CONC) .OR. EXCHR) GO TO 71	AM547
	AM548
C PRINT MOLAR CONCENTRATIONS AND REACTION CONVERSION RATES	AM549
WRITE (6,136)	AM550
WRITE (6,154)	AM551
154 FORMAT (12X,13H(MOLES/CM**3),25X,16H(MOLE/CM**3/SEC),11X,6HNUMBER,* 7X,22H(MOLE-CM**3/GM**2/SEC),7X,11H(CGS UNITS))	AM552
DO 70 J=1,LR	AM553
70 PRX(J) = XX(J)	AM554
GO TO 72	AM555
	AM556
	AM557
C PRINT MOLAR CONCENTRATIONS AND ENERGY EXCHANGE RATES	AM558
71 WRITE (6,138)	AM559
WRITE (6,155)	AM560
155 FORMAT (12X,13H(MOLES/CM**3),25X,16H(MOLE/CM**3/SEC),11X,6HNUMBER,* 8X,21H(CAL-CM**3/GM**2/SEC),7X,11H(CGS UNITS))	AM561
	AM562
	AM563
C COMPUTE MOLAR CONCENTRATIONS	AM564
72 DO 73 I=1,LS	AM565
73 PRC(I) = SIGMA(I)*RHO	AM566
	AM567
74 DO 77 IJ=1,MAX	AM568
IF (IJ .GT. LS .OR. IJ .GT. LR) GO TO 75	AM569
FMOL = SIGMA(IJ)*MIXMW	AM570
WRITE (6,140) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,W(IJ),IJ,PRX(IJ),	AM571
* RATE(IJ)	AM572
GO TO 77	AM573

75 IF (IJ .GT. LS) GO TO 76	AM574
FMOL = SIGMA(IJ)*MIXMW	AM575
WRITE (6,141) (SPNM(I,IJ),I=1,2),PRC(IJ),FMOL,W(IJ)	AM576
GO TO 77	AM577
76 WRITE (6,142) IJ,PRX(IJ),RATE(IJ)	AM578
77 CONTINUE	AM579
WRITE (6,143) MIXMW,TXXH,CSUM	AM580
WRITE (6,156)	AM581
156 FORMAT (49X,21H(CAL-CM**3/GM**2/SEC))	AM582
	AM583
78 WRITE (6,157)	AM584
157 FORMAT (//2(4X,8HARIABLE,5X,10HDERIVATIVE,6X,9HINCREMENT,6X,14HRE	AM585
*LATIVE ERROR,4X))	AM586
L = LSP3/2	AM587
	AM588
LP = L	AM589
DO 79 I=1,L	AM590
LP = LP + 1	AM591
WRITE (6,158) (SNAM(K,I),K=1,2),F(I),RK(I),E(I),	AM592
* (SNAM(K,LP),K=1,2),F(LP),RK(LP),E(LP)	AM593
158 FORMAT (2(4X,2A4,2(4X,E12.5),5X,E12.5,5X))	AM594
79 CONTINUE	AM595
	AM596
IF (2*L .EQ. LSP3) GO TO 80	AM597
WRITE (6,159) (SNAM(K,LSP3),K=1,2),F(LSP3),RK(LSP3),E(LSP3)	AM598
159 FORMAT (70X,2A4,2(4X,E12.5),5X,E12.5)	AM599
	AM600
80 IF (.NOT. DEBUG) GO TO 82	AM601
C DEBUG OUTPUT (INTERNAL UNITS)	AM602
IF (VERSA .NE. AREAV) GO TO 83	AM603
WRITE (6,160) AA,BB,DA,D2A,DTERM	AM604
160 FORMAT (1H1,12X,2HAA,18X,2HBB,13X,15HD(AREA)/D(IVAR),8X,17HD2(AREA	AM605
*)/D(IVAR)2,8X,27H(1/AREA)*D(AREA)/D(IVAR)-AA/8X,E12.5,8X,E12.5,9X,	AM606
* E12.5,12X,E12.5,18X,E12.5)	AM607
GO TO 84	AM608
83 WRITE (6,164) AA,BB,DA,D2A,DTERM	AM609
164 FORMAT (1H1,12X,2HAA,18X,2HBB,11X,19HD(PRESSURE)/D(IVAR),4X,21HD2(AM610
*PRESSURE)/D(IVAR)2,4X,32H(1/PRESSURE)*D(PRESSURE)/D(IVAR)/8X,E12.5	AM611
*,8X,E12.5,9X,E12.5,12X,E12.5,18X,E12.5)	AM612
84 WRITE (6,161) (I,I=1,LR)	AM613
161 FORMAT (/37X,58HOMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY RE	AM614
*ACTION J//1X,7HSPECIES,55X,8HREACTION/(18X,I2,7I15))	AM615
DO 81 I=1,LS	AM616
WRITE (6,162) (SPNM(K,I),K=1,2),(CMEGA(I,J),J=1,LR)	AM617
162 FORMAT (/2X,2A4,8E15.5/(10X,8E15.5))	AM618
81 CONTINUE	AM619
	AM620
82 IF (ABS(1.-CSUM) .LE. .001) RETURN	AM621
WRITE (6,163)	AM622
163 FORMAT (7H0(OUTP),5X,19HINVALID COMPOSITION)	AM623
NEXT = .TRUE.	AM624
RETURN	AM625
	AM626
END	AM627
\$IEFTC PREDD DECK	AN001
SUBROUTINE PRED	AN002
C PERFORM ALL NECESSARY PRE-DEFIVATIVE CALCUIATIONS	AN003
	AN004
DOUBLE PRECISION DP1,DP2	AN005
	AN006

LOGICAL ALLM1,TCON,NEXT	AN007
REAL IVAR,MDOT,LKEQ,MM,N,M,MIXMW,M2	AN008
	AN009
	AN010
COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,ELIM,TCON,PHOCON,IPRCOD	AN011
COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT	AN012
COMMON/SPEC/SNAM(2,30),MW(25),W(25),STOIC(25,30),OMEGA(25,30)	AN013
COMMON/REAC/LSR(4,30),XX(30),RATE(30),LKEQ(30),DLKEQ(30),MM(30),LR	AN014
COMMON/REAT/A(30),N(30),FACT(30),B(30),M(25,30),ALLM1	AN015
COMMON/GHSC/GRT(25),HRT(25),SP(25),CPP(25),DCPR(25)	AN016
COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,P	AN017
COMMON/SABS/S1,AA,RB,S2,DA,D2A,RTPEM	AN018
	AN019
IF (TCON) GO TO 5	AN020
GO TO 1	AN021
	AN022
ENTRY PRED1	AN023
MWARN = 0	AN024
C THERMODYNAMIC PROPERTIES	AN025
1 CALL THRM (T,1.)	AN026
	AN027
ALOGRT = ALOG(RR*T)	AN028
DO 4 J=1,LR	AN029
	AN030
C REACTION RATE CONSTANT	AN031
RATE(J) = A(J)*T**N(J)*EXP(-B(J)/T)	AN032
	AN033
C LN KPO AND D(LN KEO)/DT	AN034
N1 = LSR(1,J)	AN035
N2 = LSR(2,J)	AN036
N3 = LSR(3,J)	AN037
N4 = LSR(4,J)	AN038
DELG = GRT(N3) - GRT(N2)	AN039
DELH = HRT(N3) - HRT(N2)	AN040
IF (N1 .GT. 0) GO TO 2	AN041
DELG = DELG + GRT(N4)	AN042
DELH = DELH + HRT(N4)	AN043
LKEQ(J) = -DELG - ALOGRT	AN044
DLKEQ(J) = (DELH - 1.)/T	AN045
GO TO 4	AN046
2 IF (N4 .GT. 0) GO TO 3	AN047
DELG = DELG - GRT(N1)	AN048
DELH = DELH - HRT(N1)	AN049
LKEQ(J) = -DELG + ALOGRT	AN050
DLKEQ(J) = (DELH + 1.)/T	AN051
GO TO 4	AN052
3 DELG = DELG + GRT(N4) - GRT(N1)	AN053
DELH = DELH + HRT(N4) - HRT(N1)	AN054
LKEQ(J) = -DELG	AN055
DLKEQ(J) = DELH/T	AN056
4 CONTINUE	AN057
	AN058
C MIXTURE MOLECULAR WEIGHT	AN059
5 SSUM = 0.	AN060
DO 6 I=1,LS	AN061
6 SSUM = SSUM + SIGMA(I)	AN062
MIXMW = 1./SSUM	AN063
	AN064
C ASSIGNED VARIABLE	AN065
IF (IPRCOD .GT. 2) GO TO 7	AN066
X = IVAR	AN067
IF (VERSI .EQ. TIMEV) X = DVAR	AN068
CALL CIMP (X,AVAR,DA,D2A)	AN069
GO TO 3	AN070

7	TIME = DVAR	AN071
	IF (VERSI .EQ. TIMEV) TIME = IVAR	AN072
	CALL CINP (TIME,AVAR,DA,D2A)	AN073
C	CALCULATED VARIABLE	AN074
8	IF (VERSA .EQ. AREAV) GO TO 9	AN075
	P = AVAR	AN076
	IF (V .NE. 0.) AREA = MDOT/(RHO*V)	AN077
	GO TO 10	AN078
9	AREA = AVAR	AN079
	P = RHO*RR*T/MIXMW	AN080
C	MASS FLOW RATE	AN081
	MDOT = RHO*AREA*V	AN082
10	DO 20 J=1,LR	AN083
	N1 = LSR(1,J)	AN084
	N2 = LSR(2,J)	AN085
	N3 = LSR(3,J)	AN086
	N4 = LSR(4,J)	AN087
C	THIRD BODY FACTOR	AN088
	MM(J) = 0.	AN089
	IF (N1 .NE. 0 .AND. N4 .NE. 0) GO TO 13	AN090
	IF (ALLM1) GO TO 12	AN091
	DO 11 I=1,LS	AN092
11	MM(J) = MM(J) + M(I,J)*SIGMA(I)	AN093
	GO TO 13	AN094
12	MM(J) = SSUM	AN095
13	EXP1 = RATE(J)	AN096
	EXP2 = 1.	AN097
	IF (LKEQ(J) .GT. 0.) GO TO 14	AN098
	EXP2 = EXP(-LKEQ(J)/2.)	AN099
	GO TO 15	AN100
14	EXP1 = EXP(ALOG(RATE(J)) - LKEQ(J))	AN101
C	NET REACTION CONVERSION RATE	AN102
15	IF (N1 .GT. 0) GO TO 17	AN103
	IF (N1 .LT. 0) GO TO 16	AN104
	DP1 = RATE(J)*SIGMA(N2)	AN105
	DP2 = RHO*EXP1*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2	AN106
	XX(J) = MM(J)*(DP1 - DP2)	AN107
	GO TO 20	AN108
16	DP1 = RATE(J)*SIGMA(N2)/RHO	AN109
	DP2 = EXP1*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2	AN110
	XX(J) = DP1 - DP2	AN111
	GO TO 20	AN112
17	IF (N4 .GT. 0) GO TO 19	AN113
	IF (N4 .LT. 0) GO TO 18	AN114
	DP1 = RHO*SIGMA(N1)*RATE(J)*SIGMA(N2)	AN115
	DP2 = EXP1*EXP2*SIGMA(N3)*EXP2	AN116
	XX(J) = MM(J)*(DP1 - DP2)	AN117
	GO TO 20	AN118
18	DP1 = SIGMA(N1)*RATE(J)*SIGMA(N2)	AN119
	DP2 = EXP1*SIGMA(N3)*EXP2/RHO*EXP2	AN120
	XX(J) = DP1 - DP2	AN121
	GO TO 20	AN122
19	DP1 = SIGMA(N1)*RATE(J)*SIGMA(N2)	AN123
	DP2 = EXP2*SIGMA(N3)*EXP1*SIGMA(N4)*EXP2	AN124
	XX(J) = DP1 - DP2	AN125
		AN126
		AN127
		AN128
		AN129
		AN130

20 CONTINUE	AN131
RHO2 = RHO*RHO	AN132
TCPR = 0.	AN133
DO 22 I=1,LS	AN134
	AN135
C TOTAL CP/R	AN136
TCPR = TCPR + CPR(I)*SIGMA(I)	AN137
	AN138
C NET SPECIES PRODUCTION RATE	AN139
W(I) = 0.	AN140
DO 21 J=1,LR	AN141
OMEGA(I,J) = RHO2*STOIC(I,J)*XX(J)	AN142
21 W(I) = W(I) + OMEGA(I,J)	AN143
22 CONTINUE	AN144
	AN145
C GAMMA (FROZEN)	AN146
GAMMA = TCPR/(TCPR - 1./MIXMW)	AN147
	AN148
C MACH NUMBER SQUARED	AN149
M2 = V/R*V/T*MIXMW/GAMMA	AN150
	AN151
IF (VERSA .NE. AREA V .OR. (M2 .LT. 0.9025 .OR. M2 .GT. 1.1025))	AN152
* GO TO 23	AN153
WMACH = SQRT(M2)	AN154
WRITE (6,101) WMACH	AN155
101 FORMAT (7H0(PRED),5X,7HWARNING,3X,13HMACH NUMBER =,F8.4,19H IS APP	AN156
*ROACHING 1.0)	AN157
MWARN = MWARN + 1	AN158
IF (MWARN .LT. 15) GO TO 23	AN159
WRITE (6,102)	AN160
102 FORMAT (7H0(PRED),5X,25H15 WARNINGS HAVE OCCURRED)	AN161
NEXT = .TRUE.	AN162
RETURN	AN163
	AN164
23 CALL DERV	AN165
	AN166
RETURN	AN167
END	AN168
\$IEFTC DERVV DECK	AN169
SUBROUTINE DERV	AO001
	AO002
C COMPUTE ALL DERIVATIVES WRT THE INDEPENDENT VARIABLE	AO003
	AO004
DOUBLE PRECISION DPS1,DPS2	AO005
	AO006
LOGICAL TCON,RHOCON	AO007
	AO008
REAL IVAR,MIXMW,M2	AO009
	AO010
COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,ELIM,TCON,RHOCON,IPRCOD	AO011
COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT	AO012
COMMON/SPEC/SNAM(2,30),MW(25),W(25),STOIC(25,30),OMEGA(25,30)	AO013
COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)	AO014
COMMON/DERN/F(28),ALPHA(28),BETA(28,28)	AO015
COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R	AO016
COMMON/SABS/S1,AA,BB,S2,DA,D2A,DTEFM	AO017
	AO018
EQUIVALENCE (DV,F(1))	AO019

D2ADT2(D2) = V*V*D2 + DV/V*DA	A0020
D2ADX2(D2) = (D2/V - DV*DA)/V	A0021
	A0022
DPS1 = 0.D0	A0023
DPS2 = 0.D0	A0024
DO 1 I=1,3	A0025
F(I) = 0.	A0026
1 ALPHA(I) = 0.	A0027
	A0028
DENM = RHO	A0029
IF (VERSI .NE. TIMEV) DENM = RHO*V	A0030
DO 2 I=1,LS	A0031
II = I + 3	A0032
	A0033
C DSIGMA/DIVAR	A0034
F(II) = W(I)/DENM	A0035
	A0036
C S1 FOR AA	A0037
DPS1 = DPS1 + F(II)	A0038
C S2 FOR BB	A0039
2 DPS2 = DPS2 + HRT(I)*F(II)	A0040
	A0041
S1 = MIXMW*DPS1	A0042
S2 = MIXMW*DPS2	A0043
	A0044
GAM1 = GAMMA - 1.	A0045
C BB FOR DERIVATIVES	A0046
BB = GAM1/GAMMA*S2	A0047
	A0048
C AA FOR DERIVATIVES	A0049
AA = S1 - BB	A0050
	A0051
C DAVAR/DIVAR	A0052
IF (VERSI .EQ. TIMEV .AND. IPRCOD .LE. 2) DA = V*DA	A0053
IF (VERSI .NE. TIMEV .AND. IPRCOD .GE. 3) DA = DA/V	A0054
	A0055
IF (VERSA .NE. AREAV) GO TO 4	A0056
C ASSIGNED AREA EQUATIONS	A0057
DTERM = DA/AREA - AA	A0058
T1 = 1./(M2 - 1.)	A0059
T2 = M2*T1	A0060
	A0061
C DV/DIVAR	A0062
F(1) = V*T1*DTERM	A0063
	A0064
C DRHO/DIVAR	A0065
IF (.NOT. RHOCON) F(2) = -RHO*(T2*DTERM + AA)	A0066
	A0067
C DT/DIVAR	A0068
IF (.NOT. TCON) F(3) = -T*(GAM1*T2*DTERM + BB)	A0069
	A0070
C DAREA/DIVAR WRT IVAR	A0071
IF (VERSI .EQ. TIMEV .AND. (IPRCOD .EQ. 1 .AND. V .NE. 0.)) D2A =	A0072
* D2ADT2(D2A)	A0073
IF (VERSI .NE. TIMEV .AND. IPRCOD .EQ. 3) D2A = D2ADX2(D2A)	A0074
	A0075
T3 = (D2A - DA*DA/AREA)/AREA	A0076
	A0077
	A0078

C	DSIGMA/DIVAR WRT IVAR	AO079
	DO 3 I=4,LSP3	AO080
	3 ALPHA(I) = 0.	AO081
		AO082
C	DV/DIVAR WRT IVAR	AO083
	ALPHA(1) = V*T1*T3	AO084
		AO085
C	DRHO/DIVAR WRT IVAR	AO086
	IF (.NOT. RHOCON) ALPHA(2) = -RHO*T2*T3	AO087
		AO088
C	DT/DIVAR WRT IVAR	AO089
	IF (.NOT. TCON) ALPHA(3) = -T*GAM1*T2*T3	AO090
		AO091
	GO TO 6	AO092
C	ASSIGNED PRESSURE EQUATIONS	AO093
	4 DTERM = DA/P	AO094
	T2 = -1./GAMMA	AO095
		AO096
C	DV/DIVAR	AO097
	IF (V .NE. 0.) F(1) = -DA/(RHO*V)*1.01325E+06	AO098
		AO099
C	DRHO/DIVAR	AO100
	IF (.NOT. RHOCON) F(2) = -RHO*(T2*DTERM + AA)	AO101
		AO102
C	DT/DIVAR	AO103
	IF (.NOT. TCON) F(3) = -T*(GAM1*T2*DTERM + BB)	AO104
		AO105
C	DP/DIVAR WRT IVAR	AO106
	IF (VERSI .EQ. TIMEV .AND. IPRCOD .EQ. 2) D2A = D2ADT2(D2A)	AO107
	IF (VERSI .NE. TIMEV .AND. IPRCOD .EQ. 4) D2A = D2ADX2(D2A)	AO108
		AO109
	T3 = (D2A - DA*DA/P)/P	AO110
		AO111
C	DSIGMA/DIVAR WRT IVAR	AO112
	DO 5 I=4,LSP3	AO113
	5 ALPHA(I) = 0.	AO114
		AO115
C	DV/DIVAR WRT IVAR	AO116
	IF (V .NE. 0.) ALPHA(1) = -D2A/(RHO*V)*1.01325E+06	AO117
		AO118
C	DRHO/DIVAR WRT IVAR	AO119
	IF (.NOT. RHOCON) ALPHA(2) = -RHO*T2*T3	AO120
		AO121
C	DT/DIVAR WRT IVAR	AO122
	IF (.NOT. TCON) ALPHA(3) = -T*GAM1*T2*T3	AO123
		AO124
	6 CALL PARD	AO125
		AO126
	RETURN	AO127
	END	AO128
\$IBFTC	PARD D DECK	
	SUBROUTINE PARD	AP001
		AP002
C	COMPUTE ALL MIXED PARTIAL DERIVATIVES	AP003
		AP004
	LOGICAL TCON,RHOCON	AP005
		AP006
	REAL LKEQ,MM,N,M,MIXMW,M2	AP007
		AP008

DIMENSION PXXRHO(30),PXXT(30),PXXSIG(30,25),PGSIG(25),PM2SIG(25),	AP009
* PS1SIG(25),PS2SIG(25),PAASIG(25),PBBSIG(25)	AP010
COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,ELIM,TCON,RHOCON,IPRCOD	AP011
COMMON/COND/DVAR,AREA,MDOT,P,IVAR,V,RHO,T,SIGMA(25),LS,LSP3,NEXT	AP012
COMMON/SPEC/SNAM(2,30),MW(25),W(25),STOIC(25,30),OMEGA(25,30)	AP013
COMMON/REAC/LSR(4,30),XX(30),RATE(30),LKEQ(30),DLKEQ(30),MM(30),LR	AP014
COMMON/RRAT/A(30),N(30),EACT(30),B(30),M(25,30),ALLM1	AP015
COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)	AP016
COMMON/NECC/RR,MIXMW,M2,GAMMA,TCPR,R	AP017
COMMON/SABS/S1,AA,BB,S2,DA,D2A,DTERM	AP018
COMMON/DERN/F(28),ALPHA(28),BETA(28,28)	AP019
	AP020
	AP021
DO 1 I=1,LSP3	AP022
DO 1 K=1,LSP3	AP023
1 BETA(I,K) = 0.	AP024
	AP025
DO 2 J=1,LR	AP026
DO 2 I=1,LS	AP027
2 PXXSIG(J,I) = 0.	AP028
	AP029
C XX(J) WRT RHO,T,SIGMA(I)	AP030
DO 9 J=1,LR	AP031
N1 = LSR(1,J)	AP032
N2 = LSR(2,J)	AP033
N3 = LSR(3,J)	AP034
N4 = LSR(4,J)	AP035
EXP1 = RATE(J)	AP036
EXP2 = 1.	AP037
IF (LKEQ(J) .GT. 0.) GO TO 3	AP038
EXP2 = EXP(-LKEQ(J)/2.)	AP039
GO TO 4	AP040
3 EXP1 = EXP(ALOG(RATE(J)) - LKEQ(J))	AP041
	AP042
	AP043
4 IF (N1 .GT. 0) GO TO 6	AP044
IF (N1 .LT. 0) GO TO 5	AP045
PXXRHO(J) = -MM(J)*EXP2*SIGMA(N3)*EXP1*SIGMA(N4)*EXP2	AP046
PXXT(J) = MM(J)*EXP1*RHO*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2*DLKEQ(J)	AP047
PXXSIG(J,N2) = RATE(J)*MM(J) + XX(J)/MM(J)*M(N2,J)	AP048
PXXSIG(J,N3) = -MM(J)*EXP1*RHO*EXP2*SIGMA(N4)*EXP2 + XX(J)/MM(J)*	AP049
* M(N3,J)	AP050
PXXSIG(J,N4) = -MM(J)*EXP1*RHO*EXP2*SIGMA(N3)*EXP2 + XX(J)/MM(J)*	AP051
* M(N4,J)	AP052
GO TO 9	AP053
5 PXXRHO(J) = -RATE(J)/RHO*SIGMA(N2)/RHO	AP054
PXXT(J) = EXP1*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2*DLKEQ(J)	AP055
PXXSIG(J,N2) = RATE(J)/RHO	AP056
PXXSIG(J,N3) = -EXP2*(EXP1*SIGMA(N4))*EXP2	AP057
PXXSIG(J,N4) = -EXP2*(EXP1*SIGMA(N3))*EXP2	AP058
GO TO 9	AP059
	AP060
6 IF (N4 .GT. 0) GO TO 8	AP061
IF (N4 .LT. 0) GO TO 7	AP062
PXXRHO(J) = MM(J)*SIGMA(N1)*RATE(J)*SIGMA(N2)	AP063
PXXT(J) = EXP2*MM(J)*EXP1*SIGMA(N3)*EXP2*DLKEQ(J)	AP064
PXXSIG(J,N1) = MM(J)*RHO*RATE(J)*SIGMA(N2) + XX(J)/MM(J)*M(N1,J)	AP065
PXXSIG(J,N2) = MM(J)*RHO*RATE(J)*SIGMA(N1) + XX(J)/MM(J)*M(N2,J)	AP066
PXXSIG(J,N3) = -EXP1*(EXP2*MM(J))*EXP2 + XX(J)/MM(J)*M(N3,J)	AP067
GO TO 9	

7	PXXRHO(J) = EXP1*SIGMA(N3)*EXP2/RHO*EXP2/RHO	AP068
	PXXT(J) = EXP1*SIGMA(N3)*EXP2/RHO*EXP2*DLKEQ(J)	AP069
	PXXSIG(J,N1) = RATE(J)*SIGMA(N2)	AP070
	PXXSIG(J,N2) = RATE(J)*SIGMA(N1)	AP071
	PXXSIG(J,N3) = -EXP2*EXP1*(EXP2/RHO)	AP072
	GO TO 9	AP073
8	PXXRHO(J) = 0.	AP074
	PXXT(J) = EXP1*SIGMA(N3)*EXP2*SIGMA(N4)*EXP2*DLKEQ(J)	AP075
	PXXSIG(J,N1) = RATE(J)*SIGMA(N2)	AP076
	PXXSIG(J,N2) = RATE(J)*SIGMA(N1)	AP077
	PXXSIG(J,N3) = -EXP2*(EXP1*SIGMA(N4))*EXP2	AP078
	PXXSIG(J,N4) = -EXP2*(EXP1*SIGMA(N3))*EXP2	AP079
		AP080
9	PXXT(J) = PXXT(J) + XX(J)*(N(J) + B(J)/T)/T	AP081
	GTGM1 = GAMMA*(GAMMA - 1.)	AP082
	PGAMT = 0.	AP083
C	GAMMA WRT SIGMA(I) AND MACH NUMBER SQUARED WRT SIGMA(I)	AP084
	DO 10 I=1,LS	AP085
	PGSIG(I) = GTGM1*(MIXMW - CPR(I)/TCPR)	AP086
	PM2SIG(I) = -M2*(MIXMW + PGSIG(I)/GAMMA)	AP087
10	PGAMT = PGAMT + SIGMA(I)*DCPR(I)	AP088
		AP089
C	GAMMA WRT T	AP090
	PGAMT = -GTGM1/TCPR*PGAMT	AP091
		AP092
C	MACH NUMBER SQUARED WRT V	AP093
	PM2V = 2.*V*MIXMW/(GAMMA*R*T)	AP094
C	MACH NUMBER SQUARED WRT T	AP095
	PM2T = -M2*(1./T + PGAMT/GAMMA)	AP096
		AP097
	TERM = RHO	AP098
	IF (VERSI.EQ. TIMEV) GO TO 12	AP099
	TERM = RHO/V	AP100
C	DSIGMA/DIVAR WRT V	AP101
	DO 11 II=4,LSP3	AP102
11	BETA(II,1) = -F(II)/V	AP103
		AP104
C	DSIGMA/DIVAR WRT V AND DSIGMA/DIVAR WRT T	AP105
12	DO 14 II=4,LSP3	AP106
	I = II - 3	AP107
	DO 13 J=1,LR	AP108
	BETA(II,2) = BETA(II,2) + STOIC(I,J)*PXXRHO(J)	AP109
13	BETA(II,3) = BETA(II,3) + STOIC(I,J)*PXXT(J)	AP110
	BETA(II,2) = F(II)/RHO + TERM*BETA(II,2)	AP111
14	BETA(II,3) = TERM*BETA(II,3)	AP112
		AP113
C	DSIGMA(I)/DIVAR WRT SIGMA(K)	AP114
	DO 16 II=4,LSP3	AP115
	I = II - 3	AP116
	DO 16 KK=4,LSP3	AP117
	K = KK - 3	AP118
	DO 15 J=1,LR	AP119
15	BETA(II,KK) = BETA(II,KK) + STOIC(I,J)*PXXSIG(J,K)	AP120
16	BETA(II,KK) = TERM*BETA(II,KK)	AP121
		AP122
C	S1 WRT V,RHO,T,SIGMA(I) AND S2 WRT V,RHO,T,SIGMA(I)	AP123
	PS1V = 0.	AP124
	PS1RHO = 0.	AP125
	PS1T = 0.	AP126
		AP127
		AP128

PS2V = 0.	AP129
PS2RHO = 0.	AP130
PS2T = 0.	AP131
DO 18 II=4,LSP3	AP132
I = II - 3	AP133
PS1V = PS1V + BETA(II,1)	AP134
PS1RHO = PS1RHO + BETA(II,2)	AP135
PS1T = PS1T + BETA(II,3)	AP136
PS2V = PS2V + HRT(I)*BETA(II,1)	AP137
PS2RHO = PS2RHO + HRT(I)*BETA(II,2)	AP138
PS2T = PS2T + HRT(I)*BETA(II,3) + CPR(I)*F(II)/T	AP139
PS1SIG(I) = 0.	AP140
PS2SIG(I) = 0.	AP141
DO 17 KK=4,LSP3	AP142
K = KK - 3	AP143
PS1SIG(I) = PS1SIG(I) + BETA(KK,II)	AP144
17 PS2SIG(I) = PS2SIG(I) + HRT(K)*BETA(KK,II)	AP145
PS1SIG(I) = MIXMW*(PS1SIG(I) - S1)	AP146
18 PS2SIG(I) = MIXMW*(PS2SIG(I) - S2)	AP147
PS1V = MIXMW*PS1V	AP148
PS1RHO = MIXMW*PS1RHO	AP149
PS1T = MIXMW*PS1T	AP150
PS2V = MIXMW*PS2V	AP151
PS2RHO = MIXMW*PS2RHO	AP152
PS2T = MIXMW*PS2T - S2/T	AP153
	AP154
GM1DG = (GAMMA - 1.)/GAMMA	AP155
S2OG2 = S2/(GAMMA*GAMMA)	AP156
C EB WRT V	AP157
PBBV = GM1DG*PS2V	AP158
C EB WRT RHO	AP159
PBBRHO = GM1DG*PS2RHO	AP160
C EB WRT T	AP161
PBBT = GM1DG*PS2T + S2OG2*PGAMT	AP162
	AP163
C AA WRT V	AP164
PAAV = PS1V - PBBV	AP165
C AA WRT RHO	AP166
PAARHO = PS1RHO - PBBRHO	AP167
C AA WRT T	AP168
PAAT = PS1T - PBBT	AP169
	AP170
C EB WRT SIGMA(I) AND AA WRT SIGMA(I)	AP171
DO 19 I=1,LS	AP172
PBBSIG(I) = GM1DG*PS2SIG(I) + S2OG2*PGSIG(I)	AP173
19 PAASIG(I) = PS1SIG(I) - PBBSIG(I)	AP174
	AP175
IF (VPRSA .NE. AREAV) GO TO 24	AP176
C ASSIGNED AREA EQUATIONS	AP177
T1 = 1./(M2 - 1.)	AP178
GAM1 = GAMMA - 1.	AP179
	AP180
C DV/DIVAR WRT V	AP181
BETA(1,1) = T1*(DTERM - F(1)*PM2V - V*PAAV)	AP182
C DV/DIVAR WRT RHO	AP183
BETA(1,2) = -V*T1*PAARHO	AP184
C DV/DIVAR WRT T	AP185
BETA(1,3) = -T1*(V*PAAT + F(1)*PM2T)	AP186
C DV/DIVAR WRT SIGMA(I)	AP187
DO 20 II=4,LSP3	AP188
I = II - 3	AP189
20 BETA(1,II) = -T1*(V*PAASIG(I) + F(1)*PM2SIG(I))	AP190
	AP191
IF (RHOCON) GO TO 22	AP192

C	DRHO/DIVAR WRT V	AP193
	BETA(2,1) = RHO*T1*(PAAV + T1*DTERM*PM2V)	AP194
C	DRHO/DIVAR WRT RHO	AP195
	BETA(2,2) = RHO*T1*PAARHO + F(2)/RHO	AP196
C	DRHO/DIVAR WRT T	AP197
	BETA(2,3) = RHO*T1*(PAAT + T1*DTERM*PM2T)	AP198
C	DRHO/DIVAR WRT SIGMA(I)	AP199
	DO 21 II=4,LSP3	AP200
	I = II - 3	AP201
	21 BETA(2,II) = RHO*T1*(PAASIG(I) + T1*DTERM*PM2SIG(I))	AP202
		AP203
	22 IF (TCON) RETURN	AP204
C	DT/DIVAR WRT V	AP205
	BETA(3,1) = T*(GAM1*T1*(M2*PAAV + T1*DTERM*PM2V) - PBBV)	AP206
C	DT/DIVAR WRT RHO	AP207
	BETA(3,2) = T*(GAM1*M2*T1*PAARHO - PBBRHO)	AP208
C	DT/DIVAR WRT T	AP209
	BETA(3,3) = T*(T1*(GAM1*(M2*PAAT + T1*DTERM*PM2T) - M2*DTERM*PGAMT	AP210
	*) - PBBT) + F(3)/T	AP211
C	DT/DIVAR WRT SIGMA(I)	AP212
	DO 23 II=4,LSP3	AP213
	I = II - 3	AP214
	23 BETA(3,II) = T*(T1*(GAM1*(M2*PAASIG(I) + T1*DTERM*PM2SIG(I)) - M2*	AP215
	* DTERM*PGSIG(I)) - PBBSIG(I))	AP216
		AP217
	RETURN	AP218
C	ASSIGNED PRESSURE EQUATIONS	AP219
	24 T1 = 1./(GAMMA*GAMMA)	AP220
		AP221
C	DV/DIVAR WRT V	AP222
	IF (V .NE. 0.) BETA(1,1) = -F(1)/V	AP223
C	DV/DIVAR WRT RHO	AP224
	BETA(1,2) = -F(1)/RHO	AP225
C	DV/DIVAR WRT T	AP226
	BETA(1,3) = 0.	AP227
C	DV/DIVAR WRT SIGMA(I)	AP228
	DO 25 II=4,LSP3	AP229
	25 BETA(1,II) = 0.	AP230
		AP231
	IF (RHOCN) GO TO 27	AP232
C	DRHO/DIVAR WRT V	AP233
	BETA(2,1) = -RHO*PAAV	AP234
C	DRHO/DIVAR WRT RHO	AP235
	BETA(2,2) = F(2)/RHO - RHO*PAARHO	AP236
C	DRHO/DIVAR WRT T	AP237
	BETA(2,3) = -RHO*(PAAT + T1*DTERM*PGAMT)	AP238
C	DRHO/DIVAR WRT SIGMA(I)	AP239
	DO 26 II=4,LSP3	AP240
	I = II - 3	AP241
	26 BETA(2,II) = -RHC*(PAASIG(I) + T1*DTERM*PGSIG(I))	AP242
		AP243
	27 IF (TCON) RETURN	AP244
C	DT/DIVAR WRT V	AP245
	BETA(3,1) = -T*PBBV	AP246
C	DT/DIVAR WRT RHO	AP247
	BETA(3,2) = -T*PBBRHO	AP248
C	DT/DIVAR WRT T	AP249
	BETA(3,3) = BB - T*(PBBT - T1*DTERM*PGAMT) + F(3)/T	AP250
C	DT/DIVAR WRT SIGMA(I)	AP251
	DO 28 II=4,LSP3	AP252
	I = II - 3	AP253

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28 BETA(3,II) = -T*(PBBSIG(I) - T1*DTERM*PGSIG(I))
      RETURN
      END
$IBFTC THRMM DECK
      SUBROUTINE THRM (T,HONLY)

C      THIS ROUTINE CALCULATES (DIMENSIONLESS) THERMODYNAMIC PROPERTIES
C      FROM POLYNOMIAL CURVE FITS

      LOGICAL NEXT

      COMMON/COND/DUM(33),LS,LSP3,NEXT
      COMMON/GHSC/GBT(25),HRT(25),SR(25),CPR(25),DCPR(25)
      COMMON/TCOF/C(7,2,25),TLOW,TMID,THI

      F(T) = A1+T*(A2+T*(A3+T*(A4+T*A5)))

      IF (T.EQ. TPREV) RETURN

      IF (0.35*TLOW.LE. T .AND. T.LE. THI) GO TO 3
      IF (T.LE. 1.20*THI) GO TO 2

      WRITE (6,100) T
100  FORMAT (7H0 (THRM),5X,5HEXTRAPOLATED VALUES RETURNED)
      NEXT = .TRUE.
      RETURN

      2 WRITE (6,101) T
101  FORMAT (7H0 (THRM),5X,7HWARNING,3X,3HT =,F8.2,16H IS OUT OF RANGE,
      * 4X,28HEXTRAPOLATED VALUES RETURNED)

C      LOCATE PROPER TEMPERATURE RANGE
      3 K = 2
      IF (T.GT. TMID) K = 1

      DO 4 I=1,LS

C      COMPUTE H/(R*T)
      A1 = C(1,K,I) + C(6,K,I)/T
      A2 = C(2,K,I)/2.
      A3 = C(3,K,I)/3.
      A4 = C(4,K,I)/4.
      A5 = C(5,K,I)/5.
      4 HRT(I) = F(T)
      IF (HONLY.EQ. 0.) RETURN

      TPREV = T
      DO 5 I=1,LS

C      COMPUTE G/(R*T)
      A1 = C(1,K,I)*(1.-ALOG(T)) + C(6,K,I)/T - C(7,K,I)
      A2 = -C(2,K,I)/2.
      A3 = -C(3,K,I)/6.
      A4 = -C(4,K,I)/12.
      A5 = -C(5,K,I)/20.
      GRT(I) = F(T)

C      COMPUTE S/R
      A1 = C(1,K,I)*ALOG(T) + C(7,K,I)
      A2 = C(2,K,I)
      A3 = C(3,K,I)/2.

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AP254
AP255
AP256
AP257
AQ001
AQ002
AQ003
AQ004
AQ005
AQ006
AQ007
AQ008
AQ009
AQ010
AQ011
AQ012
AQ013
AQ014
AQ015
AQ016
AQ017
AQ018
AQ019
AQ020
AQ021
AQ022
AQ023
AQ024
AQ025
AQ026
AQ027
AQ028
AQ029
AQ030
AQ031
AQ032
AQ033
AQ034
AQ035
AQ036
AQ037
AQ038
AQ039
AQ040
AQ041
AQ042
AQ043
AQ044
AQ045
AQ046
AQ047
AQ048
AQ049
AQ050
AQ051
AQ052
AQ053
AQ054
AQ055
AQ056
AQ057

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A4 = C(4,K,I)/3.	AQ058
A5 = C(5,K,I)/4.	AQ059
SP(I) = F(T)	AQ060
C COMPUTE CP/R	AQ061
A1 = C(1,K,I)	AQ062
A2 = C(2,K,I)	AQ063
A3 = C(3,K,I)	AQ064
A4 = C(4,K,I)	AQ065
A5 = C(5,K,I)	AQ066
CPR(I) = F(T)	AQ067
	AQ068
C COMPUTE (DCP/DT)/R	AQ069
A1 = C(2,K,I)	AQ070
A2 = 2.*C(3,K,I)	AQ071
A3 = 3.*C(4,K,I)	AQ072
A4 = 4.*C(5,K,I)	AQ073
A5 = 0.	AQ074
5 DCPR(I) = F(T)	AQ075
	AQ076
RETURN	AQ077
END	AQ078
\$IEFTC INTEE DECK	AQ079
SUBROUTINE INTE	
C SET UP AND CALL FOR INTEGRATION	AR001
	AR002
C OBTAIN SUGGESTED STEP SIZE FOR NEXT INTEGRATION STEP	AR003
	AR004
EXTENFAL PERE	AR005
	AR006
LOGICAL NEXT,ELIM	AR007
	AR008
REAL IVAR	AR009
	AR010
DIMENSION YN(33),Y(28),C(25)	AR011
	AR012
COMMON/OPTS/VFRSI,TIMEV,VERSA,AFEA,ELIM,TCON,RHOCON,IPRCOD	AR013
COMMON/COND/YNP1(33),LS,LSP3,NEXT	AR014
COMMON/SINT/HMIN,HNM1,HN,HNP1,HMAX,NH,AVH,EMAX,EPFN,JCV,KOUNT,EPFP	AR015
COMMON/PQRE/PK(28),QK(28),RK(28),E(28)	AR016
COMMON/SPEC/SNAM(2,30),MW(25),W(25),STOIC(25,30),OMEGA(25,30)	AR017
	AR018
EQUIVALENCE (IVAR,YNP1(5)),(Y,YNP1(6)),(C,YNP1(9)),(HINT,HNM1)	AR019
	AR020
C INITIAL STEPS OR RESTART	AR021
ENTRY INTI	AR022
NREST = 0	AR023
EMAX2 = EMAX/2.	AR024
EMAX56 = 5.*EMAX/6.	AR025
LSP8 = LS + 8	AR026
HNP1 = HINT	AR027
DO 3 I=1,LSP8	AR028
3 YN(I) = YNP1(I)	AR029
2 CALL CASI (HN,QK,HNP1,PK)	AR030
HN = HNP1	AR031
CALL PRED	AR032
CALL CASI (HN,PK,HNP1,QK)	AR033
HNM1 = HN	AR034
HN = HNP1	AR035
CALL PRED	AR036
	AR037
	AR038

DO 23 I=1,LS	AR039
IF (C(I) .GE. 0.) GO TO 23	AR040
WRITE (6,100)	AR041
100 FORMAT (7H0(INTE),5X,43HCOMPOSITION ERROR - NEGATIVE CONCENTRATION	AR042
*S)	AR043
NEXT = .TRUE.	AR044
RETURN	AR045
23 CONTINUE	AR046
RETURN	AR047
C PREPARE TO CONTINUE INTEGRATION	AR048
ENTRY INTC	AR049
DO 4 I=1,LSP8	AR050
4 YNP1(I) = YN(I)	AR051
CALL PRED	AR052
RETURN	AR053
C GENERAL STEP	AR054
ENTRY INTG	AR055
CALL CASG (HN,OK,HNP1,RK)	AR056
C RELATIVE ERROR IN INTEGRATION STEP	AR057
ERRN = ERROR(Y,RK,E,JCV,HNP1)	AR058
C TEST FOR RESTART CONDITIONS	AR059
IF (ERRN .LE. EMAX .OR. HNP1 .GT. HMIN) GO TO 7	AR060
WRITE (6,101) IVAR, (SNAM(J,JCV),J=1,2),HNM1,HN,HNP1	AR061
101 FORMAT (7H0(INTE),5X,7HRESTART,10X,22HINDEPENDENT VARIABLE =,E13.5	AR062
*,2X,11H(CGS UNITS),5X,23HCONTROLLING VARIABLE =,2A4//51X,6HH(N-1)	AR063
*,17X,4HH(N),17X,6HH(N+1)/48X,3(E12.5,10X)//51X,6HK(N-1),17X,4HK(N)	AR064
*,17X,6HK(N+1),16X,6HE(N+1))	AR065
DO 5 I=1,LSP8	AR066
IF (I .GT. LSP3) GO TO 5	AR067
WRITE (6,102) (SNAM(J,I),J=1,2),PK(I),OK(I),RK(I),E(I)	AR068
102 FORMAT (30X,2A4,4(10X,E12.5))	AR069
5 YNP1(I) = YN(I)	AR070
NH = NH + 2	AR071
C STOP AFTER 10 RESTARTS	AR072
IF (NREST .LT. 10) GO TO 6	AR073
WRITE (6,103)	AR074
103 FORMAT (7H0(INTE),5X,25H10 RESTARTS HAVE OCCURRED)	AR075
NEXT = .TRUE.	AR076
RETURN	AR077
6 NREST = NREST + 1	AR078
HMIN = HMIN/2.	AR079
HNP1 = HMIN	AR080
GO TO 2	AR081
7 HNM1 = HN	AR082
HN = HNP1	AR083
DO 8 I=1,LSP8	AR084
IF (I .GT. LSP3) GO TO 8	AR085
PK(I) = OK(I)	AR086
OK(I) = RK(I)	AR087
8 YN(I) = YNP1(I)	AR088
CALL PRED	AR089
C TEST FOR NEGATIVE CONCENTRATIONS	AR090
DO 9 I=1,LS	AR091
IF (C(I) .GE. 0.) GO TO 9	AR092
WRITE (6,100)	AR093
NEXT = .TRUE.	AR094
RETURN	AR095
	AR096
	AR097
	AR098
	AR099
	AR100
	AR101

9	CONTINUE	AR102
C	OPTIONAL AUTOMATIC ELIMINATIONS	AR103
	IF (ELIM) CALL AUTO	AR104
		AR105
		AR106
C	GET STEP SIZE FOR NEXT INTEGRATION STEP	AR107
	KOUNT = 0	AR108
	IF (ERRN .GE. EMAX2) GO TO 10	AR109
	IF (HN .GE. HMAX) RETURN	AR110
	CALL SEARCH (PERR,EMAX,HN,HNP1,HMAX)	AR111
	RETURN	AR112
10	IF (ERRN .LE. EMAX56) RETURN	AR113
	IF (HN .LE. HMIN) RETURN	AR114
	CALL SEARCH (PERR,EMAX,HMIN,HNP1,HN)	AR115
	RETURN	AR116
		AR117
	END	AR118
\$IEFTC CASMM DECK		
	SUBROUTINE CASM	AS001
C	CHOOSE (1) INITIAL STEP (RESTART) FORMULA	AS002
C	(2) GENERAL STEP FORMULA	AS003
		AS004
		AS005
C	SET UP AUGMENTED MATRIX	AS006
		AS007
C	COMPUTE INCREMENTS	AS008
	DOUBLE PRECISION A	AS009
		AS010
	REAL IVAR	AS011
		AS012
	COMMON/OPTS/VERSI,TIMEV,VERSA,AREAV,ELIM,TCON,RHOCON,IPRCOD	AS013
	COMMON/COND/DVAR,ARFA,MDCT,P,IVAR,Y(28),LS,LSP3,NEXT	AS014
	COMMON/DERN/F(28),ALPHA(28),BETA(28,28)	AS015
	COMMON/MATX/A(28,29)	AS016
		AS017
	EQUIVALENCE (VN1,Y(1))	AS018
		AS019
	DATA FPS/0.0001/	AS020
		AS021
	ENTRY CASI (HN,OK,HN1,RK)	AS022
	DIMENSION OK(28),RK(28)	AS023
		AS024
		AS025
C	INITIAL STEP OR RESTART	AS026
	INGEN = 1	AS027
	JK = 0	AS028
10	F1 = 0.	AS029
	F2 = HN1	AS030
	F3 = HN1/2.	AS031
	F4 = F3	AS032
	GO TO 2	AS033
		AS034
	ENTRY CASG (HN,OK,HN1,RK)	AS035
C	GENERAL STEP	AS036
	INGEN = 2	AS037
	JK = 0	AS038
20	F1 = HN1*HN1/((2.*HN1 + HN)*HN)	AS039
	F2 = HN1*(HN1 + HN)/(2.*HN1 + HN)	AS040
	F3 = HN1	AS041
	F4 = F2	AS042
		AS043

2 LSP4 = LSP3 + 1	AS044
DO 4 I=1,LSP3	AS045
DO 3 J=1,LSP3	AS046
3 A(I,J) = -F4*BETA(I,J)	AS047
A(I,I) = 1.D0 + A(I,I)	AS048
IF (DABS(A(I,I)) .GE. EPS) GO TO 4	AS049
IF (JK .GE. 3) GO TO 4	AS050
JK = JK + 1	AS051
HN1 = 2.*((1. - EPS)/BETA(I,I))	AS052
GO TO (10,20),INGEN	AS053
4 A(I,LSP4) = F1*QK(I) + F2*(F(I) + ALPHA(I)*F3)	AS054
CALL LESV (RK)	AS055
VN = Y(1)	AS056
DO 5 I=1,LSP3	AS057
5 Y(I) = Y(I) + RK(I)	AS058
IVAR = IVAR + HN1	AS059
IF (VERSI .EQ. TIMEV) GO TO 6	AS060
DVAR = DVAR + 2.*HN1/(VN + VN1)	AS061
RETURN	AS062
6 DVAR = DVAR + (VN + VN1)/2.*HN1	AS063
RETURN	AS064
END	AS065
\$IBFTC LESVV DECK	AS066
SUBROUTINE LESV (K)	AS067
	AS068
	AS069
	AT001
	AT002
C THIS ROUTINE IS A GENERAL DOUBLE PRECISION LINEAR EQUATION SOLVER	AT003
C IN THIS PROGRAM IT IS USED TO COMPUTE THE INCREMENTS K(I)	AT004
	AT005
DOUBLE PRECISION A,S,TS,B	AT006
	AT007
LOGICAL NEXT	AT008
	AT009
REAL K	AT010
	AT011
DIMENSION S(28),K(28)	AT012
	AT013
COMMON/COND/DUMMY(34),N,NEXT	AT014
COMMON/MATX/A(28,29)	AT015
	AT016
NP = N+1	AT017
DO 5 I=1,N	AT018
C GET SCALE FACTORS	AT019
TS = 0.D0	AT020
DO 6 J=1,N	AT021
B = DABS(A(I,J))	AT022
IF (B .GT. TS) TS = B	AT023
6 CONTINUE	AT024
IF (TS .EQ. 0.D0) GO TO 100	AT025
	AT026
C SCALE ROWS	AT027
DO 10 J=1,NP	AT028
10 A(I,J) = A(I,J)/TS	AT029
5 CONTINUE	AT030
	AT031
C BEGIN TRIANGULARIZATION	AT032
IF (N .EQ. 1) GO TO 25	AT033
NM = N-1	AT034
DO 15 J=1,NM	AT035

C	FIND MAXIMUM ELEMENT IN COLUMN J BELOW DIAGONAL	AT036
	II = J	AT037
	JP = J+1	AT038
	DO 16 I=JP,N	AT039
	IF (DABS(A(I,J)) .GT. DABS(A(II,J))) II = I	AT040
16	CONTINUE	AT041
	IF (II .EQ. J) GO TO 20	AT042
C	INTERCHANGE ROWS II AND J	AT043
	DO 17 L=J,NP	AT044
	TS = A(II,L)	AT045
	A(II,L) = A(J,L)	AT046
17	A(J,L) = TS	AT047
		AT048
C	ZERO COLUMN J BELOW DIAGONAL	AT049
20	DO 18 I=JP,N	AT050
	TS = A(I,J)/A(J,J)	AT051
	IF (TS .EQ. 0.D0) GO TO 18	AT052
	DO 19 L=JP,NP	AT053
19	A(I,L) = A(I,L) - TS*A(J,L)	AT054
18	CONTINUE	AT055
15	CONTINUE	AT056
		AT057
C	BACK SUBSTITUTE	AT058
25	TS = A(N,N)	AT059
	IF (DABS(TS) .LT. 1.D-10) WRITE (6,102)	AT060
102	FORMAT (7H0(LESV),5X,11HSINGULARITY)	AT061
	S(N) = A(N,NP)/TS	AT062
	K(N) = S(N)	AT063
	IF (N .EQ. 1) RETURN	AT064
	DO 26 I=2,N	AT065
	M = NP - I	AT066
	TS = A(M,M)	AT067
	IF (DABS(TS) .LT. 1.D-10) WRITE (6,102)	AT068
	B = A(M,NP)	AT069
	MP = M+1	AT070
	DO 27 L=MP,N	AT071
27	B = B - A(M,L)*S(L)	AT072
	S(M) = B/TS	AT073
26	K(M) = S(M)	AT074
30	CONTINUE	AT075
	RETURN	AT076
		AT077
100	WRITE (6,101) I	AT078
101	FORMAT (7H0(LESV),3X,3HROW,I4,39H OF THE COEFFICIENT MATRIX IS ALL	AT079
	1 ZEROS)	AT080
	DO 50 I=1,N	AT081
50	WRITE (6,103) (A(I,J), J=1,NP)	AT082
103	FORMAT (1H1,8F16.6/(1X,8E16.6))	AT083
	NEXT = .TRUE.	AT084
	RETURN	AT085
		AT086
		AT087
	END	AU001
\$IEPTC	ERRORR DECK	AU002
	FUNCTION ERROR (Y,RK,E,JC,H)	AU003
C	COMPUTE THE RELATIVE ERROR IN AN INTEGRATION STEP OF SIZE H	AU004
C	DETERMINE THE CONTROLLING VARIABLE	AU005
	DOUBLE PRECISION DNP1,DN,DNM1,C,ABSY	AU006
		AU007
		AU008

DIMENSION Y(28),RK(28),E(28)	AU009
COMMON/COND/DUM1(33),LS,LSP3,NEXT	AU010
COMMON/SINT/HMIN,HNM1,HN,HNP1,HMAX,NH,AVH,EMAX,ERRN,JCV,KOUNT,ERRP	AU011
COMMON/PQRE/PK(28),QK(28),DUM2(56)	AU012
COMMON/SKIP/NEGL(25),I1,I2,IT	AU013
	AU014
	AU015
C = (H + HN)/(HN + HNM1)	AU016
FAC1 = ABS(H*H/(2.*H + HN)*(2.*H - HN)/(H + HN + HNM1))	AU017
	AU018
ERROR = -1.	AU019
DO 4 I=1,LSP3	AU020
E(I) = 0.	AU021
IF (ABS(RK(I)) .EQ. 0.) GO TO 4	AU022
ABSY = ABS(Y(I))	AU023
IF (ABSY .EQ. 0.) GO TO 4	AU024
DNP1 = RK(I)/H	AU025
DN = QK(I)/HN	AU026
DNM1 = PK(I)/HNM1	AU027
FAC2 = DABS((DNP1 - DN) - C*(DN - DNM1))	AU028
C CHECK FOR CATASTROPHIC SUBTRACTION	AU029
IF (FAC2 .LE. ABS(DNP1)*1.0E-04) GO TO 5	AU030
E(I) = FAC1*(FAC2/ABSY)	AU031
5 IF (I .LE. 3 .OR. IT .EQ. 0) GO TO 3	AU032
II = I - 3	AU033
C SKIP NEGLECTED SPECIES	AU034
DO 2 J=1,IT	AU035
IF (NEGL(J) .EQ. II) GO TO 4	AU036
2 CONTINUE	AU037
3 IF (E(I) .LE. ERROR) GO TO 4	AU038
ERROR = E(I)	AU039
JC = I	AU040
4 CONTINUE	AU041
	AU042
RETURN	AU043
END	AU044
\$IBFTC PERRR DECK	
FUNCTION PERR (H)	AV001
	AV002
C THIS ROUTINE PREDICTS THE ERROR WHICH CAN BE EXPECTED FROM A	AV003
C STEP OF SIZE H	AV004
	AV005
DOUBLE PRECISION SUM	AV006
	AV007
DIMENSION Y(28),RK(28),E(28)	AV008
	AV009
COMMON/COND/DUM(5),YN(28),LS,LSP3,NEXT	AV010
COMMON/SINT/HMIN,HNM1,HN,HNP1,HMAX,NH,AVH,EMAX,ERRN,JCV,KOUNT,ERRP	AV011
COMMON/DERN/F(28),ALPHA(28),BETA(28,28)	AV012
COMMON/PQRE/PK(28),QK(28),DUM1(56)	AV013
	AV014
C = H/(2.*H + HN)	AV015
C0 = H/2.	AV016
C1 = F/HN	AV017
C2 = H + HN	AV018
PERR = 0.	AV019
	AV020
DO 2 I=1,LSP3	AV021
RK(I) = C0*(QK(I)/HN + F(I))	AV022

2 E(I) = C*(C1*OK(I) + C2*(F(I) + ALPHA(T)*H))	AV023
C0 = C*C2	AV024
DO 4 I=1,LSP3	AV025
SUM = 0.D0	AV026
DO 3 J=1,LSP3	AV027
IF (J .EQ. I) GO TO 3	AV028
SUM = SUM + BETA(I,J)*RK(J)	AV029
3 CONTINUE	AV030
RK(I) = (E(I) + C0*SUM)/(1. - C0*BETA(I,I))	AV031
4 CONTINUE	AV032
	AV033
	AV034
DO 6 I=1,LSP3	AV035
SUM = 0.D0	AV036
DO 5 J=1,LSP3	AV037
5 SUM = SUM + BETA(I,J)*RK(J)	AV038
RK(I) = E(I) + C0*SUM	AV039
6 Y(I) = YN(I) + RK(I)	AV040
	AV041
PERR = ERROR(Y,RK,E,JC,H)	AV042
	AV043
RETURN	AV044
END	AV045
\$IEFTC AUTOO DECK	
SUBROUTINE AUTO	AW001
	AW002
C AUTOMATIC ELIMINATION FROM ERROR CONSIDERATIONS OF SPECIES WITH	AW003
C NON-REPRESENTATIVE ERRORS	AW004
	AW005
REAL MEDIAN	AW006
	AW007
DIMENSION ERROR(25),EE(25)	AW008
	AW009
COMMON/COND/DUM1(33),LS,LSP3,NEXT	AW010
COMMON/PQRE/DUM2(84),E(28)	AW011
COMMON/SKIP/NEGL(25),I1,I2,IT	AW012
	AW013
EQUIVALENCE (EE(1),E(4))	AW014
	AW015
I2 = 0	AW016
M = LS - I1	AW017
IF (M .LE. 3) RETURN	AW018
	AW019
K = 0	AW020
DO 3 I=1,LS	AW021
IF (I1 .EQ. 0) GO TO 2	AW022
DO 1 J=1,I1	AW023
IF (I .EQ. NEGL(J)) GO TO 3	AW024
1 CONTINUE	AW025
2 K = K + 1	AW026
ERROR(K) = EE(I)	AW027
3 CONTINUE	AW028
	AW029
N = M/2 + 1	AW030
	AW031
DO 5 NN=1,N	AW032
EMX = ERROR(NN)	AW033
I = NN	AW034
NI = NN + 1	AW035
DO 4 II=NI,M	AW036
IF (ERROR(II) .LE. EMX) GO TO 4	AW037
FMX = ERROR(II)	AW038
I = II	AW039

4	CONTINUE	AW040
	ERROR(I) = FRROR(NN)	AW041
	ERROR(NN) = EMX	AW042
5	CONTINUE	AW043
	MEDIAN = ERROR(N)	AW044
	CUTOFF = 15.*MEDIAN	AW045
		AW046
		AW047
		AW048
	DO 8 I=1,LS	AW049
	IF (I1 .EQ. 0) GO TO 7	AW050
	DO 6 J=1,I1	AW051
	IF (I .EQ. NEGL(J)) GO TO 8	AW052
6	CONTINUE	AW053
7	IF (EE(I) .LE. CUTOFF) GO TO 8	AW054
	I2 = I2 + 1	AW055
	K = I1 + I2	AW056
	NEGL(K) = I	AW057
8	CONTINUE	AW058
	IT = I1 + I2	AW059
		AW060
	RETURN	AW061
	END	
\$IEFTC	CUBSS DECK	
	SUBROUTINE CUES (X,Y,N)	AX001
		AX002
		AX003
	DIMENSION X(N),Y(N)	AX004
	DIMENSION A(40),B(40),C(40)	AX005
	DIMENSION S(40),T(40),U(40)	AX006
		AX007
	COMMON/AFUN/C1,C2,C3,C4,ITPSZ,ELM,ETA,DIAM,VISC,BFTA	AX008
		AX009
	EQUIVALENCE (A(1),U(1)),(B(1),T(1)),(C(1),S(1))	AX010
		AX011
	F(X) = ((A1*X + A2)*X + A3)*X + A4	AX012
	DF(X) = (3.*A1*X + 2.*A2)*X + A3	AX013
	D2F(X) = 6.*A1*X + 2.*A2	AX014
		AX015
	G(A) = 1./(1. - A**ETA)	AX016
	DG(B) = ETA/FLM*TERM** (ETA-1.)*B*B	AX017
	D2G(C,D,E) = C*(ETA - 1. + 2.*ETA*TERM**ETA*D)/E	AX018
		AX019
C	FROM INPUT TABLE COMPUTE COEFFICIENTS FOR CUBIC SPLINE INTERPOLATION	AX020
C	AND DIFFERENTIATION	AX021
	CON1 = .33333333	AX022
	CON2 = .16666667	AX023
	DXI = X(2) - X(1)	AX024
	DYI = Y(2) - Y(1)	AX025
	DI = DYI/DXI	AX026
	S(1) = CON1*DXI	AX027
	T(1) = CON2*DXI	AX028
	U(1) = DI - (((Y(3)-Y(1))/(X(3)-X(1))) + DI)/2.	AX029
	NM = N-1	AX030
	DO 2 I=2,NM	AX031
	DXIM = DXI	AX032
	DYIM = DYI	AX033
	DIM = DI	AX034
	DXI = X(I+1) - X(I)	AX035
	DYI = Y(I+1) - Y(I)	AX036
	DI = DYI/DXI	AX037
	S(I) = CON1*(DXIM + DXI)	AX038
	T(I) = CON2*DXI	

2	U(I) = DI - DIM	AX039
	S(N) = CON1*DXI	AX040
	U(N) = (DI + (DYI+DYIM)/(DXI+DXIM))/2. - DI	AX041
		AX042
	DO 3 I=1,NM	AX043
	TT = T(I)	AX044
	T(I) = T(I)/S(I)	AX045
	U(I) = U(I)/S(I)	AX046
	S(I+1) = S(I+1) - TT*T(I)	AX047
3	U(I+1) = U(I+1) - TT*U(I)	AX048
	U(N) = U(N)/S(N)	AX049
		AX050
	A(N) = U(N)	AX051
	DO 4 J=1,NM	AX052
	I = N-J	AX053
4	A(I) = U(I) - T(I)*A(I+1)	AX054
		AX055
	DO 5 I=1,NM	AX056
	DXI = X(I+1) - X(I)	AX057
	DYI = Y(I+1) - Y(I)	AX058
	B(I) = DYI/EXI - CON2*(A(I+1)-A(I))*DXI	AX059
5	C(I) = Y(I+1) - CON2*A(I+1)*DXI*DXI - B(I)*X(I+1)	AX060
	RETURN	AX061
		AX062
	ENTRY CIMP (XI,YI,DY,D2Y)	AX063
	GO TO (66,10,11,13),ITPSZ	AX064
		AX065
C	COMPUTE Y, DY/DX, D2Y/DX2 FROM CUBIC SPLINE COEFFICIENTS	AX066
66	DO 6 I=1,NM	AX067
	IF (X(I) .LE. XI .AND. XI .LE. X(I+1)) GO TO 7	AX068
6	CONTINUE	AX069
	WRITE (6,100) XI,X(1),X(N)	AX070
100	FORMAT (7H0(CIMP),5X,3HXI=,F13.5,17H IS OUT OF RANGE/10X,5HX(1)=,	AX071
1	F13.5,5X,5HX(N)=,F13.5)	AX072
		AX073
7	DXI = X(I+1) - X(I)	AX074
	A1 = (A(I+1)-A(I))/DXI/6.	AX075
	AIX = A(I)*X(I+1)	AX076
	AXI = A(I+1)*X(I)	AX077
	A2 = (AIX - AXI)/DXI/2.	AX078
	AIX = AIX*X(I+1)	AX079
	AXI = AXI*X(I)	AX080
	A3 = (AXI - AIX)/DXI/2. + B(I)	AX081
	AIX = AIX*X(I+1)	AX082
	AXI = AXI*X(I)	AX083
	A4 = (AIX - AXI)/DXI/6. + C(I)	AX084
		AX085
	YI = F(XI)	AX086
	DY = DF(XI)	AX087
	D2Y = D2F(XI)	AX088
	RETURN	AX089
		AX090
C	COMPUTE Y, DY/DX, D2Y/DX2 FROM INPUT POLYNOMIAL	AX091
10	A1 = C1	AX092
	A2 = C2	AX093
	A3 = C3	AX094
	A4 = C4	AX095
		AX096
	YI = F(XI)	AX097
	DY = DF(XI)	AX098
	D2Y = D2F(XI)	AX099
	RETURN	AX100
		AX101

C	COMPUTE Y, DY/DX, D2Y/DX2 FROM INPUT SPECIAL FUNCTION	AX102
C	EXCEPTIONAL CASE AT X=0	AX103
	11 IF (XI .EQ. 0.) GO TO 12	AX104
	TERM = XI/ELM	AX105
	YI = G(TERM)	AX106
	DY = DG(YI)	AX107
	D2Y = D2G(DY,YI,XI)	AX108
	RETURN	AX109
	12 YI = 1.	AX110
		AX111
		AX112
C	FIT A CUBIC THROUGH THE POINTS (0.,Y1), (.05,Y2'), (.05,Y2''), AND	AX113
C	(-.10,Y3'') IN ORDER TO FIND Y1' AND Y1''	AX114
	TERM = .05/ELM	AX115
	Y2 = G(TERM)	AX116
	Y2P = DG(Y2)	AX117
	Y2PP = D2G(Y2P,Y2,.05)	AX118
	TERM = .10/ELM	AX119
	Y3 = G(TERM)	AX120
	Y3P = DG(Y3)	AX121
	Y3PP = D2G(Y3P,Y3,.10)	AX122
		AX123
	DY = (.05*(Y3PP-Y2PP)/(.10-.05)/2. - Y2PP)*.05 + Y2P	AX124
	D2Y = Y2PP - .05*(Y3PP-Y2PP)/(.10-.05)	AX125
	RETURN	AX126
		AX127
C	V=0 CASE - ASSIGNED AREA IS NOT REQUIRED	AX128
	13 YI = 1.	AX129
	DY = 0.	AX130
	D2Y = 0.	AX131
	RETURN	AX132
		AX133
		AX134
	END	
	\$IBFTC SERCH DECK	AY001
	SUBROUTINE SEARCH (F,FOFX,A,X,B)	AY002
C	THIS ROUTINE USES AN OPTIMAL SEQUENTIAL SEARCH TECHNIQUE TO FIND X	AY003
C	IN (A,B) SUCH THAT F(X) = FOFX	AY004
		AY005
C	ASSUMPTIONS	AY006
C	(1) F(X) CONTINUOUS ON THE CLOSED INTERVAL (A,B)	AY007
C	(2) FOFX IS NOT EQUAL TO ZERO	AY008
		AY009
	COMMON/SINT/DUM(10),KOUNT,FX	AY010
		AY011
	X1 = (2.*A + B)/3.	AY012
	KOUNT = 1	AY013
	F1 = F(X1)	AY014
	IF (ABS(1.-F1/FOFX) .GT. 0.0001) GO TO 2	AY015
	X = X1	AY016
	FX = F1	AY017
	RETURN	AY018
		AY019
	2 X2 = (A + 2.*B)/3.	AY020
	KOUNT = KOUNT + 1	AY021
	F2 = F(X2)	AY022
	IF (ABS(1.-F2/FOFX) .GT. 0.0001) GO TO 3	AY023
	X = X2	AY024
	FX = F2	AY025
	RETURN	AY026
		AY027

3	D1 = F1 - FOFX	AY028
	IF (D1*(FOFX-F2) .GT. 0.) GO TO 5	AY029
	IF (D1 .LT. 0.) GO TO 4	AY030
	X2 = A	AY031
	KOUNT = KOUNT + 1	AY032
	F2 = F(X2)	AY033
	IF (F2 .LT. FOFX .AND. ABS(1.-F2/FOFX) .GT. 0.0001) GO TO 5	AY034
	X = A	AY035
	FX = F2	AY036
	RETURN	AY037
4	X1 = B	AY038
	KOUNT = KOUNT + 1	AY039
	F1 = F(X1)	AY040
	IF (F1 .GT. FOFX .AND. ABS(1.-F1/FOFX) .GT. 0.0001) GO TO 5	AY041
	X = B	AY042
	FX = F1	AY043
	RETURN	AY044
5	X = (X1 + X2)/2.	AY045
	KOUNT = KOUNT + 1	AY046
	FX = F(X)	AY047
	IF (ABS(1.-FX/FOFX) .LE. 0.0001) RETURN	AY048
	IF (KOUNT .EQ. 11) RETURN	AY049
	IF ((FX-FOFX)*(FOFX-F2) .LT. 0.) GO TO 6	AY050
	X1 = X	AY051
	GO TO 5	AY052
6	X2 = X	AY053
	F2 = FX	AY054
	GO TO 5	AY055
		AY056
		AY057
		AY058
	END	AY059
\$IEFTC MATCO DECK		
SUBROUTINE MATRIX		AZ001
DOUBLE PRECISION G,X		AZ002
DOUBLE PRECISION EN,ENLN,DELN		AZ003
LOGICAL TP,HP,CONVG,TV,UV		AZ004
		AZ005
		AZ006
		AZ007
COMMON/SPECES/EN(25),ENLN(25),DELN(25),A(15,25)		AZ008
COMMON/MISC/TT,PP,CPRO,HSUBO,ENN,SUMN,ENNL,LLMT(15),BO(15)		AZ009
COMMON/INDX/TP,HP,NLM,NS,IQ1,CONVG,KMAT,IMAT		AZ010
COMMON/GHSC/GRT(25),HRT(25),SR(25),CPR(25),DCPR(25)		AZ011
COMMON/MATX/G(28,28),X(28)		AZ012
COMMON/NECC/DUM1(4),CPSUM,DUM2		AZ013
		AZ014
EQUIVALENCE (NLM,L),(TP,TV),(HP,UV)		AZ015
		AZ016
IQ2 = IQ1 + 1		AZ017
IQ3 = IQ2 + 1		AZ018
KMAT = IQ3		AZ019
IF (.NOT.CONVG.AND.TP) KMAT = IQ2		AZ020
IMAT = KMAT - 1		AZ021
C	CLEAR MATRIX STORAGES TO ZERO	AZ022
		AZ023
	DO 211 I=1,IMAT	AZ024
	DO 211 K=1,KMAT	AZ025
	G(I,K) = 0.0E0	AZ026
211	CONTINUE	AZ027
	SSS = 0.	AZ028
	HSUM = 0.	AZ029
		AZ030
		AZ031

C	BEGIN SET UP OF ITERATION MATRIX	AZ032
	KK = L	AZ033
	TM = ALOG(PF/ENN)	AZ034
	DO 65 J=1,NS	AZ035
	H = HRT(J)*EN(J)	AZ036
	F = (HRT(J) - SR(J) + ENLN(J) + TM)*EN(J)	AZ037
	SS = H-F	AZ038
	TERM1 = H	AZ039
	IF (KMAT.EQ. IQ2) TERM1 = F	AZ040
	DO 55 I = 1, L	AZ041
		AZ042
C	CALCULATE THE ELEMENTS R(I,K)	AZ043
	IF (A(I,J).EQ. 0.) GO TO 55	AZ044
	TERM = A(I,J)*EN(J)	AZ045
	DO 15 K=I, L	AZ046
	G(I,K) = G(I,K) + A(K,J)*TERM	AZ047
15	CONTINUE	AZ048
	G(I,IQ1) = G(I,IQ1) + TERM	AZ049
	G(I,IQ2) = G(I,IQ2) + A(I,J)*TERM1	AZ050
	IF (CONVG.OR.TP) GO TO 55	AZ051
	G(I,IQ3) = G(I,IQ3) + A(I,J)*F	AZ052
55	CONTINUE	AZ053
	IF (KMAT.EQ. IQ2) GO TO 64	AZ054
	IF (CONVG.OR.HP) GO TO 59	AZ055
	G(IQ2,IQ1) = G(IQ2,IQ1) + SS	AZ056
	G(IQ2,IQ2) = G(IQ2,IQ2) + HRT(J)*SS	AZ057
	G(IQ2,IQ3) = G(IQ2,IQ3) + (SR(J) - ENLN(J) - TM)*F	AZ058
	GO TO 62	AZ059
59	G(IQ2,IQ2) = G(IQ2,IQ2) + HRT(J)*H	AZ060
	IF (CONVG) GO TO 64	AZ061
	G(IQ2,IQ3) = G(IQ2,IQ3) + HRT(J)*F	AZ062
62	G(IQ1,IQ3) = G(IQ1,IQ3) + F	AZ063
64	G(IQ1,IQ2) = G(IQ1,IQ2) + TERM1	AZ064
65	CONTINUE	AZ065
	SSS = SSS + G(IQ2,IQ1)	AZ066
	HSUM = HSUM + G(IQ1,IQ2)	AZ067
	G(IQ1,IQ1) = SUMN - ENN	AZ068
C	REFLECT SYMMETRIC PORTIONS OF THE MATRIX	AZ069
	ISYM = IQ1	AZ070
	IF (HP.OR.CONVG) ISYM = IQ2	AZ071
	DO 102 I=1,ISYM	AZ072
	DO 102 J=I,ISYM	AZ073
	G(J,I) = G(I,J)	AZ074
102	CONTINUE	AZ075
C	COMPLETE THE RIGHT HAND SIDE	AZ076
	IF (CONVG) GO TO 175	AZ077
	DO 145 I=1,L	AZ078
145	G(I,KMAT) = G(I,KMAT) + B0(I) - G(I,IQ1)	AZ079
	G(IQ1,KMAT) = G(IQ1,KMAT) + ENN - SUMN	AZ080
C	COMPLETE ENERGY ROW AND TEMPERATURE COLUMN	AZ081
	IF (KMAT.EQ. IQ2) RETURN	AZ082
	IF (HP) ENERGY = HSUBO/TT - HSUM	AZ083
	G(IQ2,IQ3) = G(IQ2,IQ3) + ENERGY	AZ084
		AZ085
		AZ086
		AZ087
		AZ088
		AZ089
		AZ090
		AZ091
		AZ092
		AZ093

175	G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM	AZ094
	RETURN	AZ095
	END	AZ096
\$IEFTC	GAUSCO DECK	AZ097
	SUBROUTINE GAUSS	
C	SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS	BA001
	DOUBLE PRECISION G,X,COEFX(20),SUM,Z	BA002
	COMMON/MATX/G(28,28),X(28)	BA003
	COMMON/INDX/TP,HP,NLM,NS,IQ1,CONVG,KMAT,IMAT	BA004
	EQUIVALENCE (IUSE,IMAT)	BA005
	DATA BIGNO/1.E+38/	BA006
C	BEGIN ELIMINATION OF NNTH VARIABLE	BA007
	IUSE1=IUSE+1	BA008
6	DO 45 NN=1,IUSE	BA009
	IF (NN-IUSE) 8,83,8	BA010
83	IF (G(NN,NN)) 31,23,31	BA011
C	SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW	BA012
8	DO 18 I=NN,IUSE	BA013
	COEFX(I) = BIGNO	BA014
	IF (G(I,NN).EQ.0.) GO TO 18	BA015
	COEFX(I) = 0.	BA016
	DO 10 J=NN,IUSE1	BA017
	SUM = G(I,J)	BA018
	IF (SUM.LT.0.) SUM=-SUM	BA019
	IF (J.NE.NN) GO TO 9	BA020
	Z = SUM	BA021
	GO TO 10	BA022
9	IF (SUM.GT.COEFX(I)) COEFX(I)=SUM	BA023
10	CONTINUE	BA024
	COEFX(I) = COEFX(I)/Z	BA025
18	CONTINUE	BA026
	TEMP = BIGNO	BA027
	I=0	BA028
20	DO 22 J=NN,IUSE	BA029
	IF (COEFX(J)-TEMP) 87,22,22	BA030
87	TEMP=COEFX(J)	BA031
	I=J	BA032
22	CONTINUE	BA033
	IF (I) 28,23,28	BA034
C	INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH	BA035
C	VARIABLE FROM THE REMAINING EQUATIONS	BA036
C	INTERCHANGE EQUATIONS I AND NN	BA037
28	IF (NN-I) 29,31,29	BA038
29	DO 30 J=NN,IUSE1	BA039
	Z=G(I,J)	BA040
	G(I,J)=G(NN,J)	BA041
	G(NN,J)=Z	BA042
		BA043
		BA044
		BA045
		BA046
		BA047
		BA048
		BA049
		BA050
		BA051
		BA052
		BA053
		BA054
		BA055

30	CONTINUE	BA056
C	DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH	BA057
C	VARIABLE FROM THE REMAINING EQUATIONS	BA058
		BA059
		BA060
31	K = NN + 1	BA061
	DO 36 J = K, IUSE1	BA062
	IF (G(NN,NN).EQ.0.) GO TO 23	BA063
	G(NN,J) = G(NN,J)/G(NN,NN)	BA064
36	CONTINUE	BA065
	IF (K-IUSE1) 88,45,88	BA066
88	DO 44 I = K, IUSE	BA067
40	DO 44 J = K, IUSE1	BA068
	G(I,J) = G(I,J) - G(I,NN)*G(NN,J)	BA069
44	CONTINUE	BA070
45	CONTINUE	BA071
C	BACKSOLVE FOR THE VARIABLES	BA072
	K = IUSE	BA073
47	J = K + 1	BA074
	X(K) = 0.0D0	BA075
	SUM = 0.0	BA076
	IF (IUSE - J) 51,48,48	BA077
48	DO 50 I = J, IUSE	BA078
	SUM = SUM + G(K,I)*X(I)	BA079
50	CONTINUE	BA080
51	X(K) = G(K,IUSE1) - SUM	BA081
	K = K - 1	EA082
	IF (K) 47,151,47	BA083
23	IUSE = IUSE-1	BA084
151	RETURN	BA085
	END	BA086
		BA087
		BA088

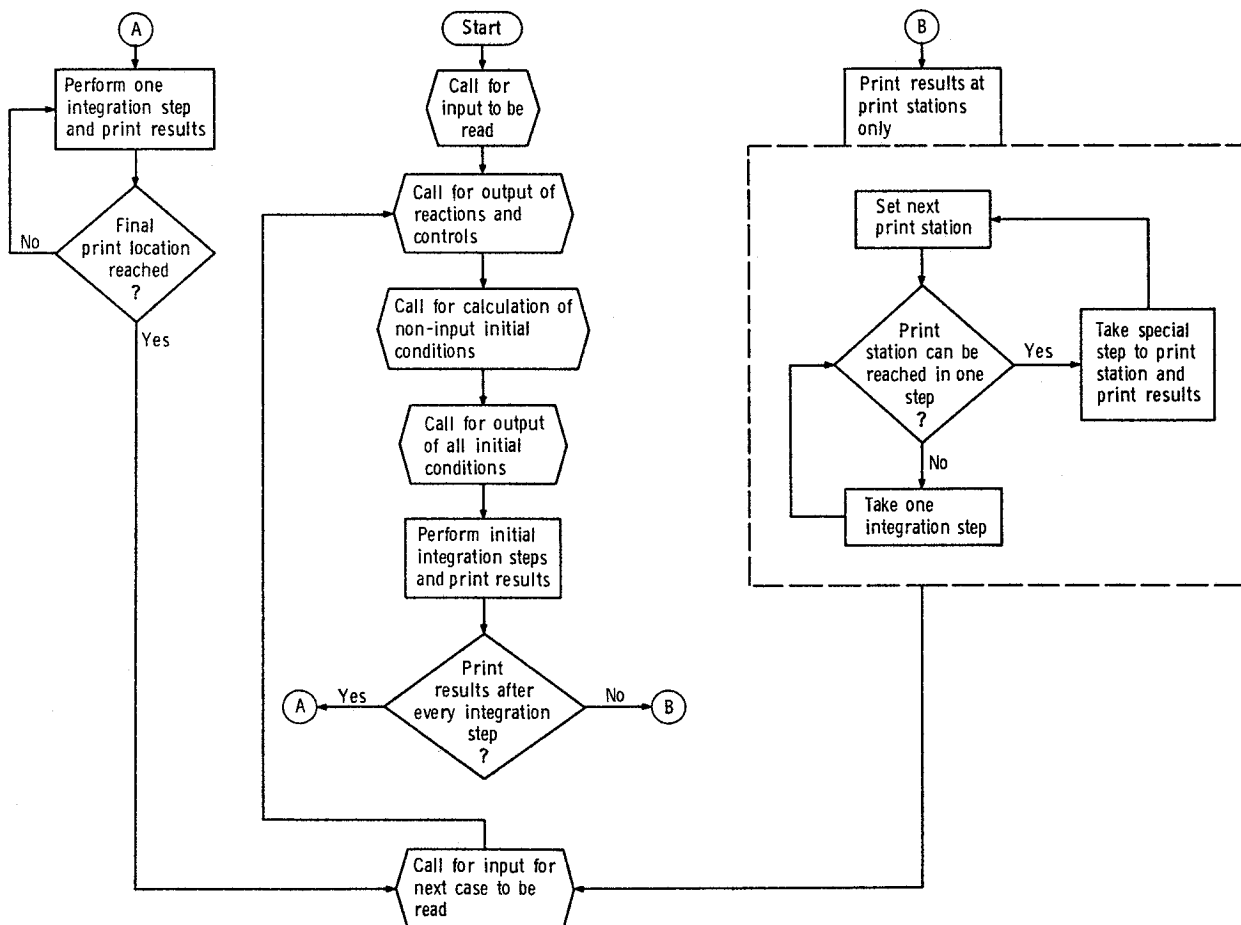


Figure 1. - Main program (GCKP).

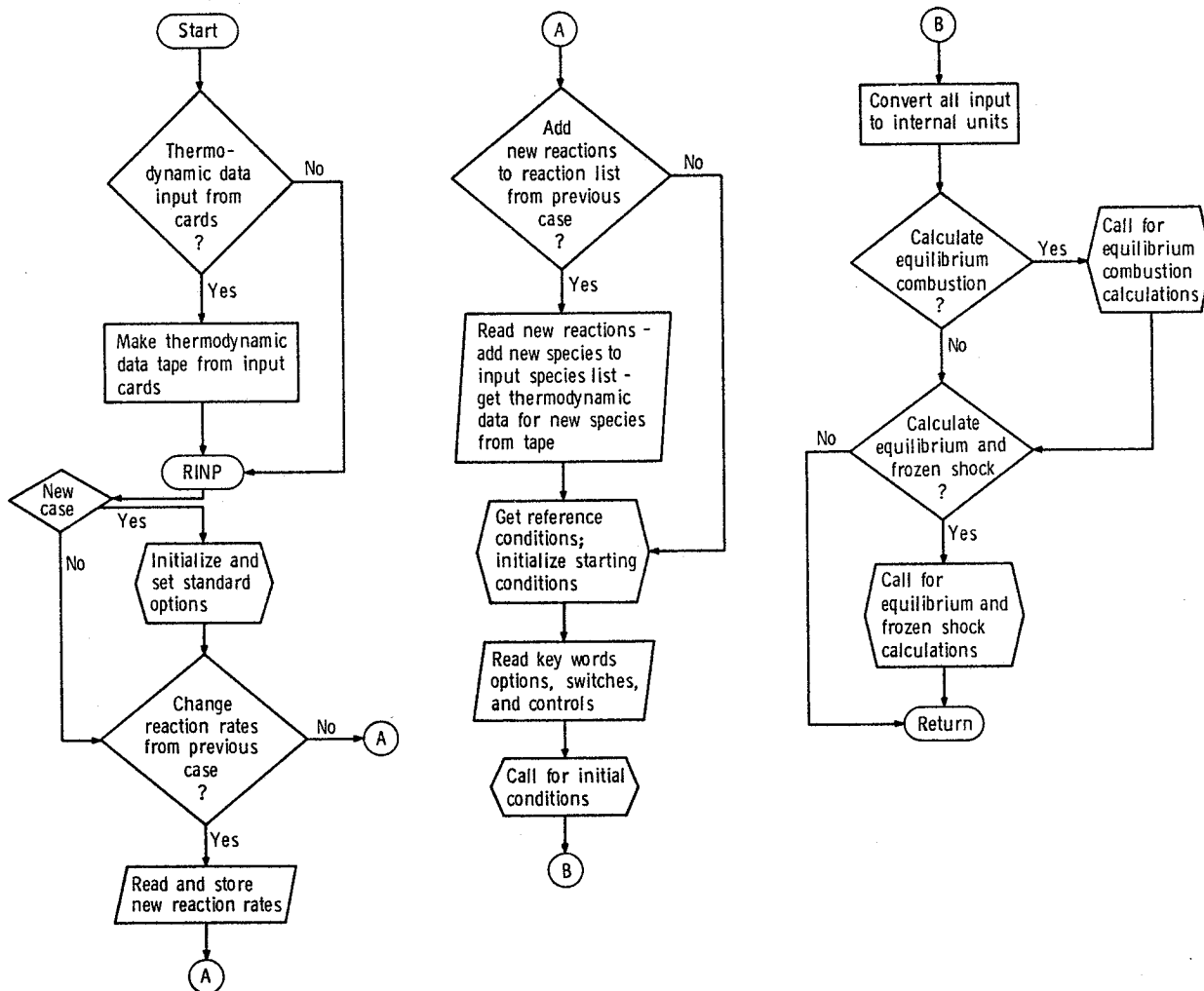


Figure 2. - Subroutine KINP.

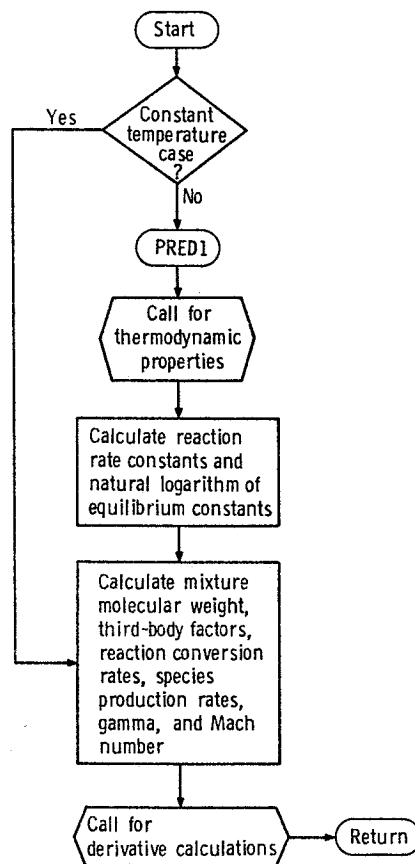


Figure 3. - Subroutine PRED.

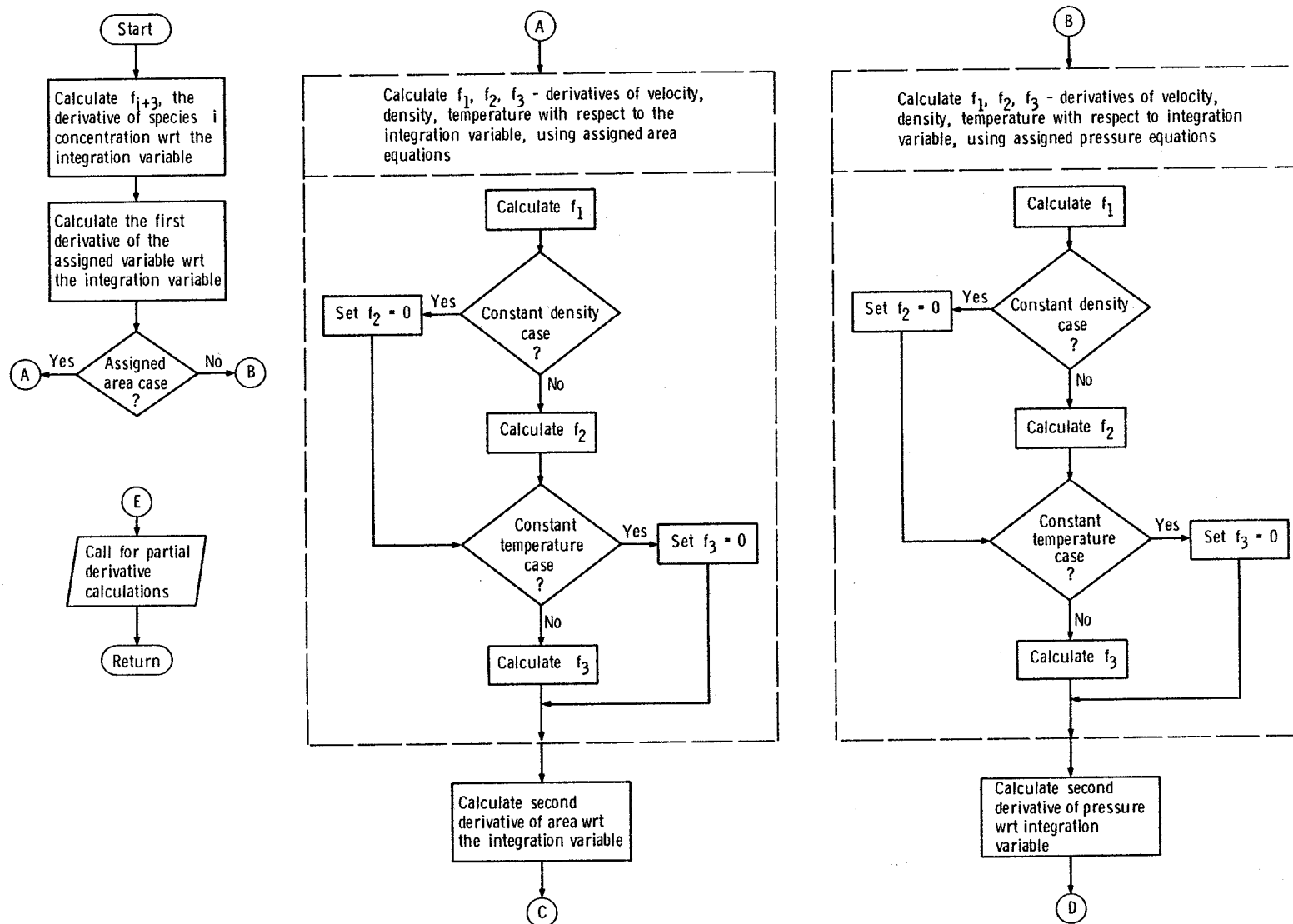


Figure 4. - Subroutine DERV.

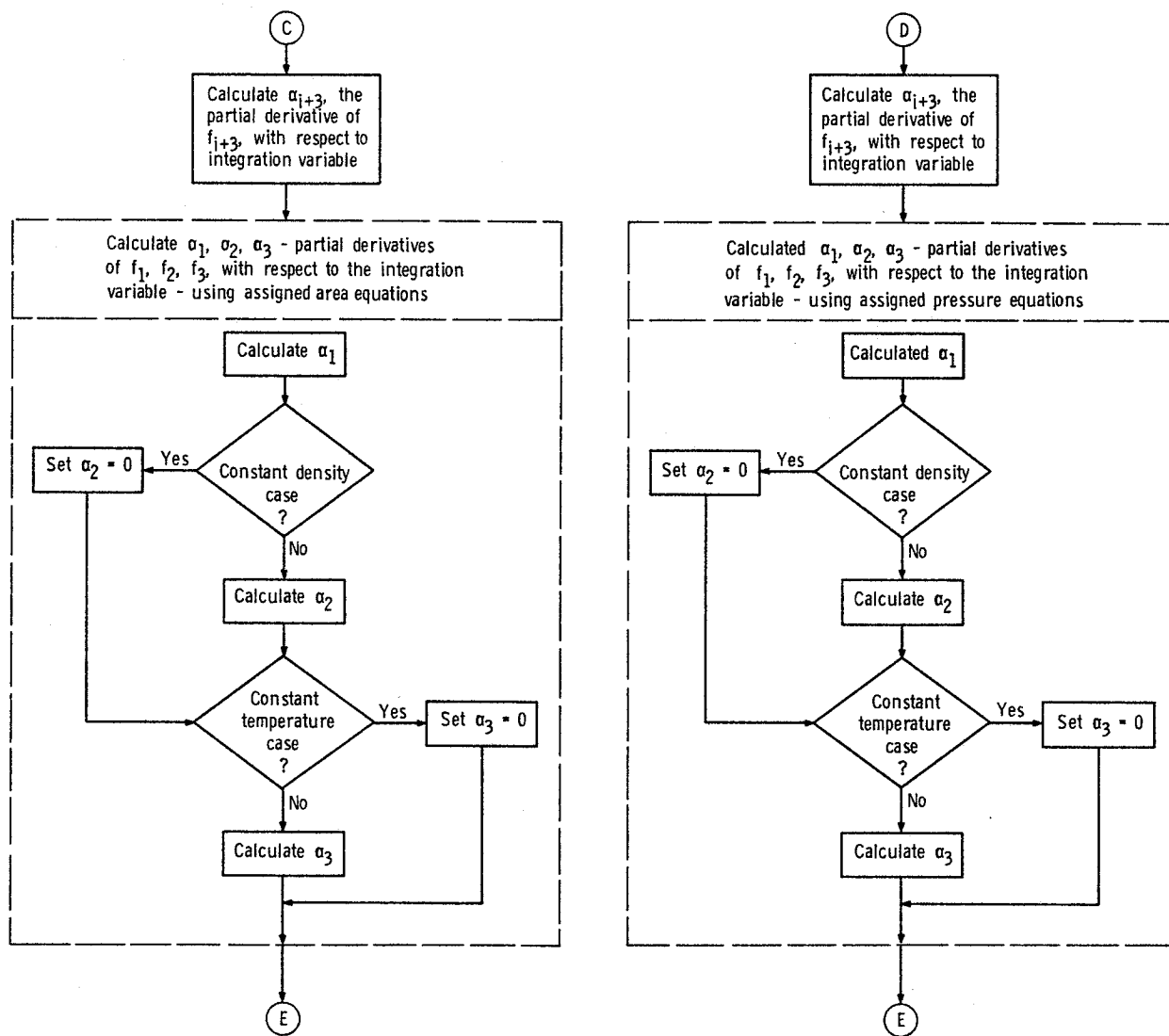


Figure 4. - Concluded.

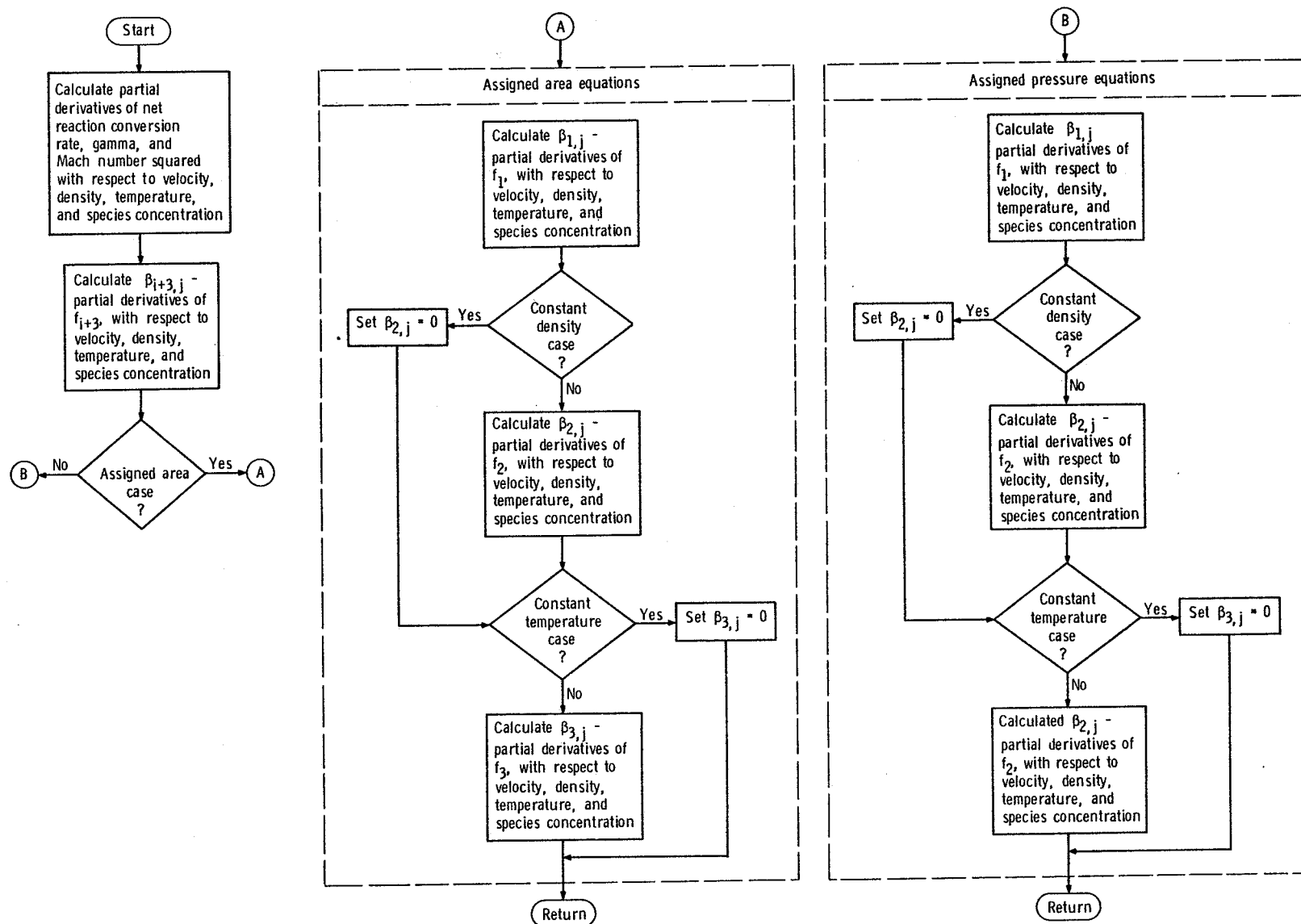
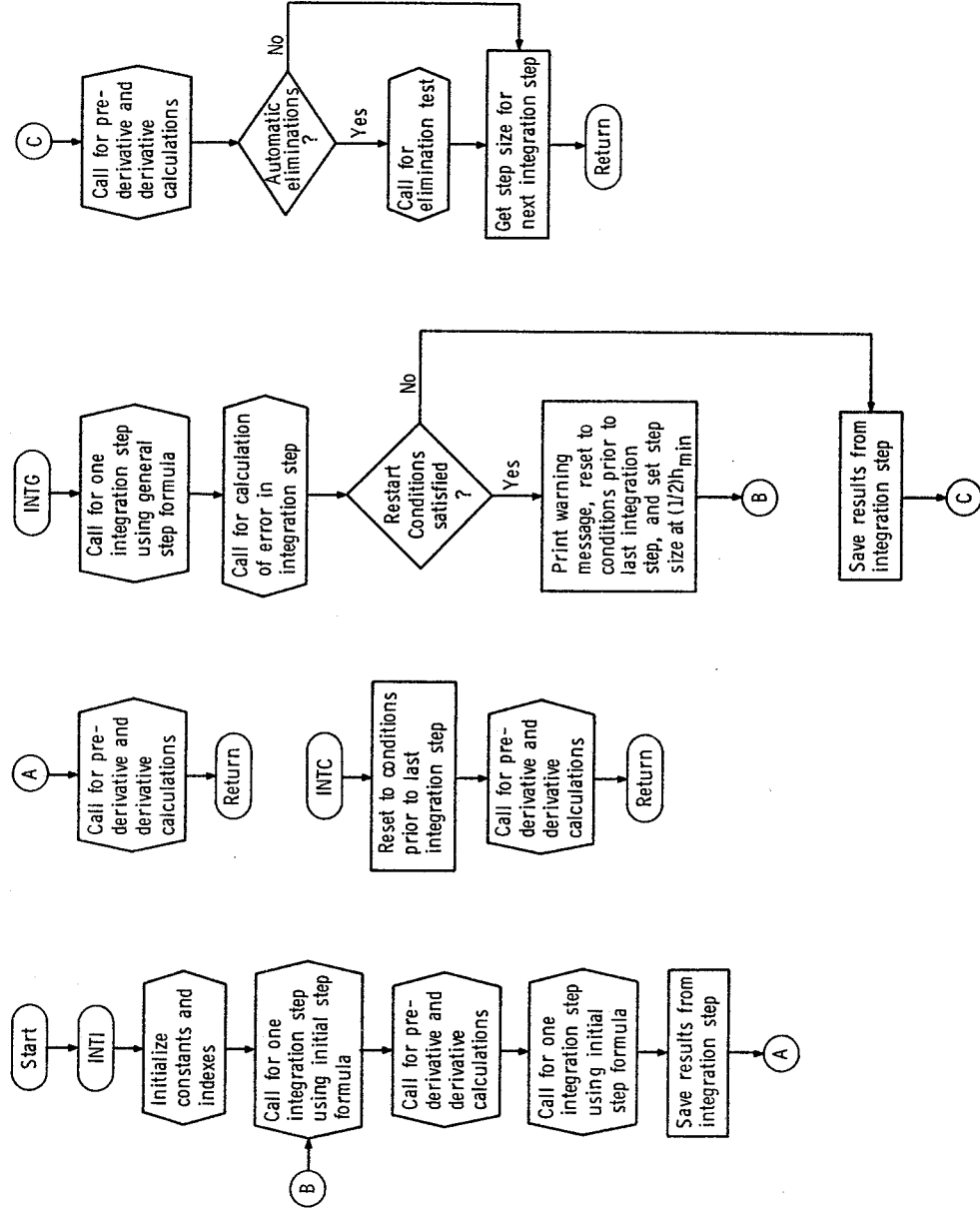


Figure 5. - Subroutine PARD.



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